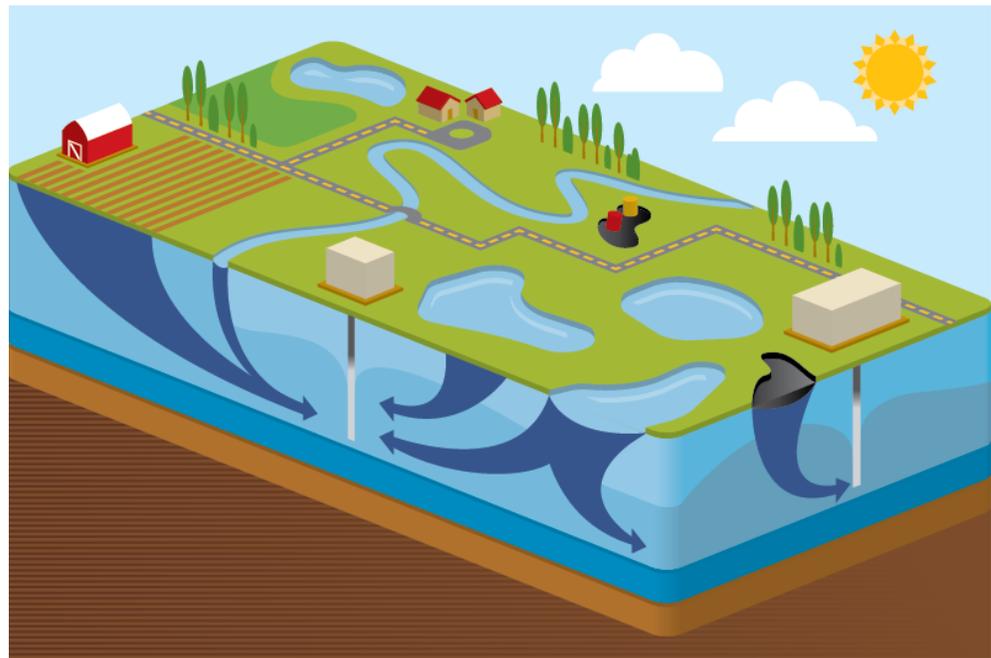


# GoldSim Contaminant Transport Module





Copyright GoldSim Technology Group LLC, 1998-2021. All rights reserved.  
GoldSim is a registered trademark of GoldSim Technology Group LLC

Primary funding for the GoldSim Contaminant Transport Module was provided by the United States Department of Energy. Additional funding was provided by the Japan Atomic Energy Agency (JAEA), and Empresa Nacional de Residuos Radioactivos, S.A. (Enresa).

GoldSim Version 14.0 (October 2021)



GoldSim Technology Group  
255 S. King Street, Suite 800  
Seattle, Washington 98104  
USA

Visit us at our web site: [www.goldsim.com](http://www.goldsim.com)  
Email us at: [software@goldsim.com](mailto:software@goldsim.com)



---

# Contents

<b>Chapter 1: Introduction</b>	<b>1</b>
<b>Chapter Overview</b> .....	<b>1</b>
In this Chapter.....	1
<b>What is the Contaminant Transport Module?</b> .....	<b>1</b>
What Makes the Program Unique? .....	3
<b>What is the Difference Between GoldSim CT and GoldSim RT?</b> .....	<b>4</b>
<b>Who Should Use the Contaminant Transport Module?</b> .....	<b>5</b>
<b>How the GoldSim Documentation is Organized</b> .....	<b>5</b>
The GoldSim Documentation Suite .....	5
How this Manual is Organized.....	6
<b>Learning to Use the Contaminant Transport Module</b> .....	<b>7</b>
<b>Conventions Used in this Manual</b> .....	<b>9</b>
<b>Activating the Contaminant Transport Module</b> .....	<b>9</b>
<b>Using Help</b> .....	<b>10</b>
<b>Technical Support, User Resources and Software Upgrades</b> .....	<b>11</b>
GoldSim Maintenance Program .....	11
Getting Technical Support .....	11
Other GoldSim Resources.....	11
<b>Chapter 2: Contaminant Transport Module Overview</b>	<b>13</b>
<b>Chapter Overview</b> .....	<b>13</b>
In this Chapter.....	13
<b>Top-Down Modeling Philosophy</b> .....	<b>14</b>
What is "Bottom-Up" Modeling?.....	14
What is "Top-Down" Modeling? .....	14
<b>Modeling Contaminant Transport Using GoldSim: Basic Concepts</b> .....	<b>16</b>
Contaminant Species.....	16
Modeling Transport Pathways .....	17
Modeling Contaminant Sources .....	19
Modeling Impacts to Receptors .....	20
<b>Features and Capabilities of Transport Pathways</b> .....	<b>20</b>
Cell Pathway Features.....	21
Aquifer Pathway Features .....	22
Pipe Pathway Features .....	23
External Pathway Features .....	24
Network Pathway Features .....	24
<b>What Does the Contaminant Transport Module Add to the GoldSim User Interface?</b> .....	<b>25</b>
<b>Building a Contaminant Transport Model in GoldSim</b> .....	<b>26</b>
Defining Species .....	27
Defining Media .....	29
Defining Pathways .....	31
Interconnecting Transport Pathways.....	33
Defining Sources.....	35
Defining Impacts to Receptors.....	36
Defining Disruptive Events.....	37
<b>Using Basic GoldSim Features in Contaminant Transport Models</b> .....	<b>38</b>
Utilizing the Basic GoldSim Elements in a Contaminant Transport Model .....	38
Representing Variability in the Contaminant Transport Module .....	38

Utilizing GoldSim's Graphical Features in a Contaminant Transport Model.....	39
<b>Where Do I Go from Here? .....</b>	<b>39</b>
Contaminant Transport Module Online Course .....	39
Contaminant Transport Example Models .....	40
<b>Chapter 3: Species and Media .....</b>	<b>41</b>
<b>Chapter Overview .....</b>	<b>41</b>
In this Chapter.....	41
<b>The Material Container .....</b>	<b>42</b>
<b>Creating and Editing Species .....</b>	<b>43</b>
Adding a New Species .....	44
Editing an Existing Species.....	46
Reordering Species .....	46
Displaying and Using Species from the ICRP Database.....	47
Removing Species.....	52
Defining Species Properties .....	52
Importing and Exporting Species Data from/to a Spreadsheet.....	58
Understanding the Browser View of the Species Element.....	62
<b>Creating and Editing Environmental Media .....</b>	<b>64</b>
Editing the Reference Fluid .....	64
Adding and Editing Fluids and Solids.....	68
Defining Fluids .....	69
Defining Solids .....	74
Entering Media Properties for Isotopes of the Same Element.....	80
Understanding the Browser View of Media Elements .....	81
Representing Spatial Variability in Media Properties .....	84
<b>Copying Material Elements Between GoldSim Model Files .....</b>	<b>85</b>
<b>Chapter 4: Transport Pathways .....</b>	<b>87</b>
<b>Chapter Overview .....</b>	<b>87</b>
In this Chapter.....	87
<b>Understanding Transport Pathways.....</b>	<b>88</b>
What is a Transport Pathway?.....	88
Types of Pathway Elements .....	88
Creating Pathway Networks.....	89
<b>Creating Mass Flux Links .....</b>	<b>90</b>
Understanding Advective Mass Flux Links .....	90
Understanding Diffusive Mass Flux Links .....	95
Understanding Direct Transfer Mass Flux Links .....	103
Understanding Precipitate Removal Mass Flux Links .....	107
Understanding Fraction of Inflows (Treatment) Mass Flux Links.....	112
Specifying the Link Type for Mass Flux Links .....	118
<b>Using Cell Pathways.....</b>	<b>119</b>
Features and Capabilities of Cells.....	120
Defining Basic Cell Properties.....	122
Defining Initial and/or Boundary Conditions for a Cell.....	126
Simulating Discrete Changes to the Mass Inventory in a Cell.....	132
Cell Pathway Outputs.....	133
Viewing a Cell in the Browser .....	135
Advective Flux Links to/from Cells.....	136
Diffusive Flux Links to/from Cells .....	139
Direct Transfer Flux Links to/from Cells.....	146
Precipitate Removal Flux Links to/from Cells.....	147
Treatment Flux Links to/from Cells.....	149

Automatically Generating Cell Networks Using the CellNet Generator.....	151
Simulating Solubility Limits in Cells.....	159
Coupling a Network of Cell Pathways to a Network of Reservoir or Pool Elements .....	163
Basic Concepts of the Cell Solution Algorithm .....	164
Saving Results for a Cell.....	173
<b>Using Aquifer Pathways .....</b>	<b>174</b>
Features and Capabilities of Aquifers .....	175
Aquifer Pathway Example: Advection, Retardation and Dispersion .....	176
Defining Basic Aquifer Properties .....	177
Simulating Suspended Solids in an Aquifer.....	185
Aquifer Pathway Outputs.....	186
Viewing an Aquifer in the Browser .....	187
Flux Links to/from Aquifers .....	188
Understanding How an Aquifer Pathway Works .....	189
Saving Results for an Aquifer.....	193
<b>Using Pipe Pathways.....</b>	<b>194</b>
Features and Capabilities of Pipes .....	195
Advective-Dispersive Transport in Pipes.....	196
Defining Basic Pipe Properties .....	198
Defining a Sorptive Coating Material for a Pipe.....	205
Simulating Storage Zones in a Pipe .....	206
Simulating Suspended Solids in a Pipe.....	212
Pipe Pathway Outputs .....	213
Viewing a Pipe in the Browser.....	213
Flux Links to/from Pipes.....	214
Simulating Time-Variable Pipe Properties .....	215
Controlling the Pipe Solution Algorithm .....	216
Summary of Limitations on the Use of Pipe Pathways.....	217
Saving Results for a Pipe .....	217
<b>Using External Pathways.....</b>	<b>219</b>
Features and Capabilities of External Pathways .....	219
General Information Flow to and from an External Pathway .....	221
Defining External Pathway Properties .....	222
Flux Links to/from External Pathways.....	228
External Pathway Outputs.....	230
Viewing an External Pathway in the Browser.....	230
Saving Results for an External Pathway .....	231
<b>Using Network Pathways.....</b>	<b>232</b>
Features and Capabilities of Network Pathways.....	232
Defining Network Pathway Properties.....	234
Defining Fracture Sets .....	241
Network Pathway Outputs .....	243
Viewing a Network Pathway in the Browser .....	243
Flux Links to/from Network Pathways .....	244
Mass Balance in a Network Pathway.....	246
Controlling the Network Pathway Solution Algorithm.....	246
Summary of Limitations on the Use of Network Pathways .....	246
Saving Results for a Network Pathway.....	246
<b>Additional Comments on the Use of Transport Pathways.....</b>	<b>247</b>
Understanding the Solution Precision.....	247
Computing Pipe and Aquifer Pathway Concentrations Accounting for Transverse Dispersion ..	249
Comparison of Aquifers and Pipes for Simulating a One-Dimensional Pathway .....	251
Manipulating Pathway Outputs.....	253
Mass Balance of Transport Media in Pathway Networks .....	253
Moving, Copying and Cloning Pathways .....	254
Placing Pathways in Conditional or Looping Containers.....	255

Simulating Looping Pathway Networks .....	256
<b>Chapter 5: Contaminant Sources</b>	<b>259</b>
<b>Chapter Overview</b> .....	<b>259</b>
In this Chapter.....	259
<b>Using Contaminant Sources</b> .....	<b>260</b>
What is a Source?.....	260
When Should You Use a Source Element?.....	261
Processes Modeled by a Source .....	261
<b>Defining a Source: Overview</b> .....	<b>263</b>
<b>Defining the Level of Containment</b> .....	<b>264</b>
<b>Defining Source Inventories</b> .....	<b>265</b>
Specifying an Inventory .....	265
<b>Associating Cells with a Source</b> .....	<b>268</b>
Defining Associated Cells.....	269
Defining Inventory Cells.....	270
Understanding the Behavior of Associated Cells.....	271
<b>Defining Barrier Failure</b> .....	<b>271</b>
Understanding Barrier Failure.....	272
Simulating Outer Barrier Failure .....	273
Simulating Inner Barrier Failure .....	276
Specifying Failure Distributions for Barriers.....	277
Controlling the Outer Barrier Failure Algorithm .....	280
Disrupting Packages Using Discrete Events .....	281
<b>Source Outputs</b> .....	<b>282</b>
<b>Instantaneously Moving Mass from a Source</b> .....	<b>282</b>
<b>Source Example Models</b> .....	<b>283</b>
Source Example #1: Barrier Failure and Solubility-Controlled Release.....	283
Source Example #2: Matrix Degradation.....	284
<b>Viewing a Source in the Browser</b> .....	<b>285</b>
<b>Saving Results for a Source</b> .....	<b>286</b>
<b>Chapter 6: Receptors</b>	<b>289</b>
<b>Chapter Overview</b> .....	<b>289</b>
In this Chapter.....	289
<b>Computing Impacts to Receptors</b> .....	<b>290</b>
<b>Defining a Receptor</b> .....	<b>290</b>
<b>Viewing a Receptor in the Browser</b> .....	<b>292</b>
<b>Saving Results for a Receptor</b> .....	<b>292</b>
<b>Chapter 7: Advanced Modeling Concepts</b>	<b>293</b>
<b>Chapter Overview</b> .....	<b>293</b>
In this Chapter.....	293
<b>Representing Spatial Variability</b> .....	<b>294</b>
Defining Spatially Variable Decay Rates.....	294
Defining Spatially Variable Media Properties .....	295
<b>Non-Linear Partitioning</b> .....	<b>297</b>
Non-Linear Partitioning Example: The Langmuir Isotherm .....	297
<b>Modeling Complex Chemical Reactions</b> .....	<b>299</b>
Modeling Higher Order Reactions .....	300
Representing Stoichiometry .....	300
Complex Reaction Example: Monod Kinetics .....	301
Competing Reactions .....	303
<b>Simulating Non-Chemical Constituents</b> .....	<b>303</b>

Bacteria and Viruses .....	304
Colloids and Particulates.....	304
Heat Transport .....	304
<b>Appendix A: Introduction to Environmental Simulation</b>	<b>307</b>
<b>Appendix Overview</b> .....	<b>307</b>
In this Appendix.....	307
<b>What is Environmental Simulation?</b> .....	<b>308</b>
<b>Carrying Out an Environmental Simulation: An Overview</b> .....	<b>308</b>
Iterative Environmental Simulation .....	309
<b>Developing a Conceptual Model</b> .....	<b>310</b>
Specifying Modeling Objectives and Defining the System .....	310
Describing Features, Processes and Events.....	311
<b>Building the Mathematical Model</b> .....	<b>312</b>
<b>Quantifying Input Parameters</b> .....	<b>312</b>
<b>Documentation and Quality Assurance</b> .....	<b>313</b>
Documenting an Environmental Simulation .....	313
Quality Assurance Procedures .....	314
<b>References</b> .....	<b>314</b>
<b>Appendix B: Details of Pathway Computations</b>	<b>315</b>
<b>Appendix Overview</b> .....	<b>315</b>
In this Appendix.....	315
<b>Cell Pathway Details</b> .....	<b>316</b>
Mass Balance Equation for Cell Pathways .....	316
Computing Concentrations in Cells .....	323
Impact of Available Porosity on Cell Pathway Behavior.....	326
Solution Algorithm for a Cell Net.....	327
<b>Pipe Pathway Details</b> .....	<b>347</b>
Governing Equations for Pipe Pathways.....	347
Solution Technique for Pipe Pathways .....	358
<b>Plume Function Details</b> .....	<b>373</b>
Calculating the Correction Factor .....	374
Relative Length Adjustment .....	374
Transverse Dispersion.....	375
Vertical Dispersion .....	376
<b>Aquifer Pathway Details</b> .....	<b>378</b>
<b>Network Pathway Details</b> .....	<b>383</b>
Developing a Transfer Matrix for a Network of Pipes.....	383
<b>References</b> .....	<b>383</b>
<b>Appendix C: Implementing External (DLL) Pathways</b>	<b>385</b>
<b>Appendix Overview</b> .....	<b>385</b>
In this Appendix.....	385
<b>Details of External Pathway Functions</b> .....	<b>386</b>
Special Requirements for External Pathway Function Input/Output Argument Lists.....	386
Passing Mass Between GoldSim and the External Pathway Function.....	387
Additional Comments on External Pathway Functions.....	387
<b>External Pathway Function Example</b> .....	<b>388</b>
<b>Appendix D: Network Pathway File Format</b>	<b>393</b>
<b>Appendix Overview</b> .....	<b>393</b>
<b>Fracture Network File Format</b> .....	<b>394</b>

<b>Appendix E: Details of Source Computations</b>	<b>399</b>
<b>Appendix Overview</b> .....	<b>399</b>
In this Appendix.....	399
<b>Barrier Failure Distributions</b> .....	<b>400</b>
Immediate Failure Distribution .....	400
Uniform Failure Distribution .....	400
Weibull Failure Distribution .....	400
Exponential Failure Distribution.....	401
User-Defined and Table Failure Distributions .....	401
<b>Combining Failure Modes</b> .....	<b>401</b>
<b>Computing Exposure Rates</b> .....	<b>402</b>
Understanding Exposure.....	402
Calculating the Exposure Rate for a Source.....	403
<b>Glossary of Terms</b>	<b>407</b>
<b>Index</b>	<b>411</b>

---

# Chapter 1: Introduction

**A journey of a thousand miles begins with a single step.**

**Confucius**

## Chapter Overview

GoldSim is a user-friendly, highly graphical, object-oriented program for carrying out dynamic, probabilistic simulations to support management and decision-making in engineering, science and business.

The GoldSim Contaminant Transport Module is a program extension to GoldSim which allows you to probabilistically simulate the release, transport, and fate of mass (e.g., contaminants) within complex engineered and/or natural environmental systems.

Each of the GoldSim modules has a separate User's Guide describing its capabilities and features. This document provides a complete description of the features and use of the GoldSim Contaminant Transport Module.



**Note:** This document only describes the Contaminant Transport Module, and assumes that you are familiar with the basic capabilities of GoldSim (described in the **GoldSim User's Guide**).

---

## In this Chapter

This introductory chapter discusses the following topics:

- What is the Contaminant Transport Module?
- What is the Difference Between GoldSim CT and GoldSim RT?
- Who Should Use the Contaminant Transport Module?
- How the GoldSim Documentation is Organized
- Learning to Use the Contaminant Transport Module
- Conventions Used in this Manual
- Activating the Contaminant Transport Module
- Using Help
- Technical Support, User Resources and Software Upgrades

## What is the Contaminant Transport Module?

The GoldSim Contaminant Transport Module is a program extension to the GoldSim simulation framework that allows you to dynamically model mass transport within complex engineered and/or natural environmental systems. A

*mass transport model* is a mathematical representation of an actual system (e.g., the subsurface environment near a waste disposal site) which can be used to simulate (and hence predict) the release, transport (movement) and ultimate fate of mass within the system. The "mass" that is typically simulated is that of chemical contaminants that have been accidentally released or intentionally disposed of within the system. As a result, such models are often referred to as *contaminant transport models*.

It is important to understand that unlike the basic GoldSim framework itself, which is quite generic, the Contaminant Transport Module was specifically designed to be applied to a particular class of problems: those associated with modeling the transport (movement) of mass (typically contaminants) through a system (e.g., soils, surface water bodies, groundwater). As such, the fundamental output produced by the GoldSim Contaminant Transport Module consists of predicted masses and mass transfer rates at specified locations within the system, and predicted concentrations within environmental media (e.g., water, soil, air) throughout the system. If desired, concentrations in environmental media can be converted to doses and/or health risks to receptors by assigning appropriate conversion factors.

More specifically, the Contaminant Transport Module can be used to represent the following processes:

- **Release of mass (e.g., contaminants)** from specified sources, taking into account 1) the failure of engineered barriers and containers (if any) in which the contaminants are disposed; and 2) degradation of any materials in which the contaminants are bound (e.g., grout, metal, glass).
- **Transport of mass** through multiple transport pathways within an environmental system (e.g., aquifers, streams, lakes, soil atmosphere).

The transport pathways can consist of any number of transport and storage media (e.g., water, air, soil), and a variety of transport mechanisms can be directly simulated, including 1) advection via fluids (e.g., movement of dissolved constituents in water); 2) advection via solids (e.g., movement of constituents adsorbed to and/or mixed with solids via erosion and transport of contaminated soil); 3) diffusion through fluids; 4) advection and diffusion of contaminated particulates suspended in fluids; and 5) diffusion across boundary layers associated with adjacent fluids (e.g., transport across the air-water interface). Transport processes can incorporate solubility constraints and partitioning of contaminants between the media present in the system, and can include the effects of chemical reactions and decay processes.

In broad terms, you could use these capabilities to apply GoldSim and the Contaminant Transport Module to a wide variety of environmental problems, such as:

- investigation of the transport and fate of contaminants (or natural components) in aquifers, wetlands, lakes and other complex ecosystems;
- evaluation of the performance of existing or proposed disposal facilities and hazardous waste sites;
- investigation of the potential impact of engineered facilities such as mines, power plants, and processing facilities on the environment; and

- simulation of the transport and fate of pharmaceuticals and other compounds within biological systems (e.g., physiologically-based pharmacokinetic modeling).

Having described the types of problems that it can be applied to, it is also important to highlight the manner in which GoldSim can represent these kinds of systems (and the limitations that imposes).

When environmental systems are modeled numerically, it is necessary to discretize space into finite volumes. For example, if you were modeling a lake, you could discretize the lake vertically (into layers) and horizontally (into areal sections), forming a three-dimensional grid of finite volumes. The question then becomes: how much discretization is appropriate? At one extreme, the lake could be represented using tens of layers and hundreds of areal sections (resulting in thousands of finite volumes). At the other extreme, the entire lake could be represented using a single finite volume.

The level of spatial discretization that is appropriate in such a case is a function of a number of things, the most important being the level of “mixing” that can be assumed. Representing the lake as a single finite volume is equivalent to assuming that the entire lake is always (instantaneously) well-mixed. Representing the lake as four vertical layers (four finite volumes) is equivalent to assuming that each layer is always (instantaneously) well-mixed.

When building a model, it is critical to give considered thought to the appropriate level of spatial discretization. For a case like a lake, it is often easy to do so (e.g., it is often quite appropriate to assume well-mixed conditions over a layer or even the entire water body). For other problems it is more difficult. For example, for systems involving advection and/or diffusion along a path (e.g., flow through an aquifer), a coarse level of discretization (e.g., representing an entire aquifer using a small number of finite volumes) can result in unrealistic spreading of the mass (a phenomenon known as numerical dispersion; as will be discussed, GoldSim has special features to deal with this specific issue.)

As a general rule, GoldSim is designed to represent systems at a relatively low level of discretization (tens or hundreds of finite volumes). That is, referring to the example above, a lake might be represented in GoldSim as two well-mixed layers (finite volumes), rather than many hundreds or thousands of finite volumes. This is not to say that GoldSim is not capable of representing systems at a higher level of spatial discretization. But it is not designed to be used in this way.

One other point is also important to understand regarding the Contaminant Transport Module. The Contaminant Transport Module itself is used to model the movement of mass through the system. This movement is typically the result of movement of media (e.g., water) through the system. This results in the advection of mass through the system (e.g., dissolved in the moving water). The key point here is that the Contaminant Transport Module requires the media flows through the system as input. That is, it solves equations based on specified media flow rates. It does not itself solve for the media flow rates. This means that you are required to create a flow model (using the basic GoldSim framework) that produces the media flow rates that can subsequently be used by the Contaminant Transport Module.

There are a variety of existing tools for simulating the transport and fate of contaminants in the environment. Because the Contaminant Transport Module utilizes all the capabilities of the GoldSim simulation framework, however, it has several unique features not present in traditional contaminant transport simulation tools:

## **What Makes the Program Unique?**

- *The program is extremely flexible*, allowing it to be applied to nearly any kind of environmental system. The software is designed in a modular manner such that model details can be added by directly entering functional relationships or linking user-defined functions or subroutines (e.g., finite difference flow models) into the program. Hence, a GoldSim application can be very simple or extremely complex, and the complexity of the model can readily evolve as more knowledge regarding the system is obtained.
- *The program is highly graphical*, such that you can literally draw a picture of the environmental system that you wish to simulate. You can also add graphics, explanatory text, and hyperlinks to document your model.
- *Uncertainty in processes, parameters and future events can be explicitly represented*. Uncertainty in processes and parameters can be represented by specifying model inputs as probability distributions. The impact of uncertain events (e.g., earthquakes, floods, sabotage) can also be directly represented by specifying the occurrence rates and consequences of such “disruptive events”.

These features, in combination with powerful contaminant transport capabilities, make the GoldSim Contaminant Transport Module a unique and powerful simulation tool.

## What is the Difference Between GoldSim CT and GoldSim RT?

There are two versions of the Contaminant Transport Module that can be added to GoldSim: the CT Module and the RT Module. Your copy of GoldSim will have neither, one, or the other (but not both), depending on your license. The CT (Contaminant Transport) Module provides all of the features and capabilities that most contaminant transport modelers will need. The RT (Radionuclide Transport) Module includes all of the capabilities of CT, along with several additional features designed to facilitate simulation of radioactive waste disposal facilities and the fate and transport of radionuclides in the environment.

In particular, the RT module provides the following additional features:

- The RT Module allows decay chains (daughter products) to be simulated (one species can be specified to transform into one or more others). To support modeling of radioactive decay chains, the RT Module also allows you to link to an extensive database of radionuclide decay data (based on a standard reference provided by the International Commission for Radiation Protection).
- The CT Module allows you to specify decay rates, but you cannot specify reaction (daughter) products.
- The RT Module provides a special element called a Source. The Source element can be used to simulate the complex release mechanisms of contaminants from engineered systems. This is particularly useful when simulating the behavior of proposed or existing waste disposal facilities, which have as part of their design engineered packages or containers in which the waste is placed prior to disposal.
- The RT Module has a special type of pathway element called a Network Pathway. Network pathways provide a computationally

efficient way to simulate large, complex networks of one-dimensional conduits in order to describe contaminant transport through fractured rock systems.

- The RT Module has a special type of element called a CellNet Generator. CellNet Generators provide an easy way to rapidly create two-dimensional Cell networks.
- The RT Module provides an option to utilize a large built-in database of radionuclide decay data (species, decay rates and daughter products). The data is based on the International Commission for Radiation Protection (ICRP)'s Publication 107. The feature allows you to view over 1300 radionuclides (along with their corresponding stable elements) and to selectively include some of these radionuclides in your simulation.

## Who Should Use the Contaminant Transport Module?

The GoldSim Contaminant Transport Module is intended for use by engineers, scientists, researchers and students who are interested in understanding and predicting the migration of mass (e.g., contaminants) in environmental systems.

The software itself, although relatively complex, can be mastered by anyone familiar with the basic functions of a personal computer and the Windows operating system. The key requirements for applying the Contaminant Transport Module are a clear understanding of the physical system being modeled and a basic understanding of uncertainty analysis and probability theory:

- Because the software was designed to be extremely flexible, it intentionally imposes few constraints on the inputs that you define. Hence, it is your responsibility to ensure that the system being defined is consistent and realistic. As a result, the most important requirement for applying the program is that you have a clear understanding of the features, processes, and events controlling the behavior of the system to be modeled. This should include a good understanding of the fundamentals of contaminant transport modeling.
- Although GoldSim can be run in a deterministic manner (i.e., no specified uncertainty in input parameters), one of the key features of GoldSim is its ability to explicitly represent such uncertainty through the use of probability distributions. In order to do so, the user must have at least a basic understanding of the representation and propagation of uncertainty. Appendix A of the **GoldSim User's Guide** provides a brief primer on this topic, along with suggestions for further reading.

## How the GoldSim Documentation is Organized

### The GoldSim Documentation Suite

The Contaminant Transport Module is a specialized extension to the basic GoldSim simulation framework. The document you are reading only describes the GoldSim Contaminant Transport Module, and assumes that you are familiar with the basic capabilities of GoldSim.

### How this Manual is Organized

The basic capabilities of GoldSim are described in the **GoldSim User's Guide**. That document provides a complete description of the features and capabilities of the GoldSim simulation framework.

This document is organized into seven chapters and five appendices. The chapters describe *what the program can do* and *how you make the program work*. Most users, however, will also want to understand *how the program carries out the calculations* (i.e., what equations are being solved, what are the basic assumption inherent in these equations, and what numerical techniques are being used to solve the equations). This information is provided in the appendices.

The seven chapters are as follows:

- **Chapter 1: Introduction.** The remainder of this chapter discusses the information required for you to get started using the GoldSim Contaminant Transport Module, including conventions used in the manual, activating the module, using online help, and obtaining technical support.
- **Chapter 2: Contaminant Transport Module Overview.** This chapter provides an overview of the features and capabilities of the Contaminant Transport Module, summarizes the specialized contaminant transport elements, and outlines the steps required to build a contaminant transport model in GoldSim.
- **Chapter 3: Species and Media.** This chapter describes how you define the basic building blocks of a contaminant transport simulation: 1) the contaminant species which are to be simulated; and 2) the environmental media (e.g., water, soil) in which these species are transported and stored.
- **Chapter 4: Transport Pathways.** This chapter describes the fundamental component of a contaminant transport simulation, the transport pathway. A contaminant transport model is constructed by defining multiple transport pathways and linking them together into a network.
- **Chapter 5: Contaminant Sources.** This chapter describes how you can introduce mass into a transport pathway network by defining one or more "sources", whose contaminant release rates are a function of a variety of user-defined properties.
- **Chapter 6: Receptors.** This chapter describes how concentrations in various media within transport pathways can be converted to impacts (e.g., health risk, dose) to specified receptor groups (e.g., adults, children, farmers).
- **Chapter 7: Advanced Modeling Concepts.** This chapter discusses a number of advanced contaminant transport topics, and will be of particular interest to experienced modelers. It includes discussions of modeling complex (high-order) chemical reactions, nonlinear chemical partitioning, spatial variability, and the dynamic linking of GoldSim to external codes (e.g., flow models, geochemical equilibrium models).

The five appendices contain the following information:

- **Appendix A: Introduction to Environmental Simulation.** This appendix provides an overview of basic environmental simulation concepts, and is primarily intended for novice contaminant transport modelers.

- **Appendix B: Details of Pathway Computations.** This appendix presents the theoretical basis and mathematical details of the transport pathways.
- **Appendix C: Implementing External (DLL) Pathways.** This appendix provides instructions for those users who wish to directly link external contaminant transport codes into a GoldSim transport pathway network.
- **Appendix D: Network Pathway File Format.** This appendix describes the file format which can be used to import data from a discrete fracture network model into a specialized pathway in GoldSim that allows you to simulate complex pathways in fractured rock.
- **Appendix E: Details of Source Computations.** This appendix presents the theoretical basis and mathematical details of the contaminant sources.

The manual also includes a Glossary of Terms and an Index.

As will be discussed below, nearly all of the information available in the printed documentation can also be accessed via an extensive online help system.

## Learning to Use the Contaminant Transport Module

Although GoldSim's intuitive interface will tempt you to simply dive in and start playing with the software, you are strongly discouraged from doing so, even if you are an experienced modeler. Spending some time up front (by following the steps outlined below) is the quickest and most effective way to understand the software's features and capabilities and start building models using the GoldSim Contaminant Transport Module.

1. **Learn how to use the basic GoldSim framework first.** In order to use the Contaminant Transport Module, you must first have a basic understanding of the GoldSim framework. You cannot learn the extension without first learning the basic concepts underlying framework. At a minimum, you should take the GoldSim Tutorial. The Tutorial is available from the GoldSim splash screen, and can also be accessed from the main GoldSim menu (**Help | Tutorial...**).

In addition to the Tutorial, a free "hands-on" online training Course (titled "Introduction to GoldSim") is available that will provide you with a thorough understanding of the key concepts on which GoldSim is based and all of the fundamentals required to build complex models of nearly any kind of system. (Note, however, that the Course only discusses basic GoldSim and does not discuss the Contaminant Transport Module; a separate Course, discussed below, covers the Contaminant Transport Module). Because the Course is quite thorough, it will likely take as long as 40 hours to complete. Of course, if you are already somewhat familiar with simulation (and/or have a strong quantitative background), you may in fact be able to cover the material in considerably less than 40 hours. You can find the Course here: <https://www.goldsim.com/Courses/BasicGoldSim/>.

2. **Read "Contaminant Transport Module Overview".** This section of GoldSim Help (equivalent to Chapter 2 of the Contaminant Transport Module User's Guide) provides an introduction to and a "quick tour" of the GoldSim Contaminant Transport Module. It presents the basic

concepts of how contaminant transport is simulated in GoldSim, provides an overview of the features and capabilities of the program, summarizes the specialized elements associated with the module, and outlines the steps required to build a contaminant transport model for an environmental system.

3. **Take the Online “GoldSim Contaminant Transport Module” Training Course.** The quickest and most effective way to learn how to use the Contaminant Transport Module is to take the free “hands-on” online “Contaminant Transport Module” online Course. This will provide you a thorough understanding of the key concepts on which the GoldSim Contaminant Transport Module is based and all of the fundamentals required to build complex models of nearly any kind of system. That is, it does not simply focus on the mechanics of using the Contaminant Transport Module; just as importantly, it explains the fundamental concepts underlying contaminant transport modeling in general.

Note that prior to taking this Course (which focuses solely on the Contaminant Transport Module), you should first take the “Introduction to GoldSim Course” discussed above (item 1).

Because the Course is quite thorough, it will likely take as long as 40 hours to complete. Of course, if you are already familiar with contaminant transport modeling, you may in fact be able to cover the material in considerably less than 40 hours.

You can take the Course at your own pace (and the site will remember where you last left off).

You can find the Course here:

<https://www.goldsim.com/Courses/ContaminantTransport/>.

4. **Open and explore the Example Files.** When you install GoldSim, a number of example models are installed with the program. (You can quickly access these files by selecting **File|Open Example...** from the main GoldSim menu, and look in a subfolder named Contaminant Transport Examples). These examples are referenced in the Help system and User’s Guide where the element is introduced. These example model files are an excellent way to begin to experiment with the Contaminant Transport Module.
5. **Download Example Files from the Model Library.** The GoldSim website contains a Model Library with a number of models illustrating how GoldSim can be used for particular applications. The library includes a number of Contaminant Transport models. These models tend to be more complex than the simple example files found in the Contaminant Transport Examples folder, but are still relatively simple.
6. **Browse the User’s Guide or Help System.** GoldSim has a large number of features, and you will not discover all of them by experimenting with simple example models. To fully utilize GoldSim’s powerful features, browse through the User’s Guide, using the index and table of contents as your guide. Each section of the User’s Guide is heavily cross-referenced, so it is easy to just jump around. Note that the Help system contains all of the contents of the User’s Guide, with the exception of the technical appendices.
7. **Request your free one hour web-based training session.** When you purchase GoldSim, you are entitled to a free one hour, live web-based

training session in which one of our analysts provides an interactive training session via the Internet and telephone. You are strongly encouraged to take advantage of this free training, during which our analysts can provide an introduction to both the basic GoldSim framework and the Contaminant Transport Module.

8. **Contact us with questions.** When you purchase GoldSim, you are entitled to one year of free support. This does not include assistance in building and debugging your models, but it does include answering questions on how to use GoldSim's features, so feel free to contact us! The best way to do so is through the GoldSim Help Center.

## Conventions Used in this Manual

The following conventions are used in this manual:

Convention	Description
<i>Important Terms</i>	New and important terms are presented in <i>bold italics</i> . These terms all appear in the Glossary of Terms at the end of the document.
File   Open...	Menus and menu selections are separated by a vertical bar. <u>F</u> ile   <u>O</u> pen... means "Access the File menu and choose Open"
CTRL+C	Key combinations are shown using a "+" sign.. CTRL+C means press the Control and C keys simultaneously.
	<b>Warning:</b> This means watch out! Warnings typically alert you to potential pitfalls and problems that may occur if you perform (or fail to perform) a certain action.
	<b>Note:</b> Notes highlight important information about a particular concept, topic or procedure, such as limitations on how a particular feature can be used, or alternative ways of carrying out an action.

In describing various mouse actions, the following conventions are used:

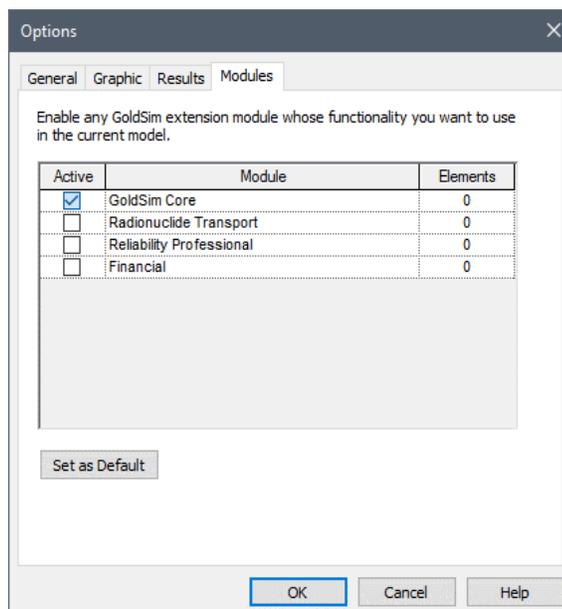
Mouse Action	Definition
Click	Press and release the left mouse button once.
Double-click	Press and release the left mouse button twice in rapid succession.
Right-click	Press and release the right mouse button once.
Drag	Press the left mouse button, and while keeping it depressed, move the cursor to another location, then release the button.

## Activating the Contaminant Transport Module

In order to access the features and capabilities of the Contaminant Transport Module, either the CT Module or the RT Module must first be activated on your machine. Your copy of GoldSim will have neither, one, or the other (but not both), depending on your license.

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4).

You can determine which (if any) of the Contaminant Transport Modules is activated on your machine by selecting **Model | Options...** from the main menu, and selecting the **Modules** tab:



All extension modules that you are licensed to use appear in the dialog. If your license does not allow you to use a particular module, it will not be listed. You can activate and deactivate modules that you are licensed to use by clicking the **Active** checkbox. By default, whenever you activate GoldSim, none of the available extension modules allowed by your license will be activated. To use them, you must activate them using this dialog.



**Note:** If you try to open a file that contains elements associated with the CT or RT Module, and you are licensed to use that module but it is not currently active, GoldSim will automatically activate the module and open the file. If, however, you are not licensed to use the module, GoldSim will not open the file (and will display an error message).

If you deactivate a module (such as CT or RT), the specialized elements associated with that module will be deleted from your model (if any are present) and any menu options will be removed in the current file. If you make a module active, the various options associated with that module are made available again. If you press the **Set as Default** button, the selected modules will be activated for all new models that are created.

## Using Help

GoldSim has an extensive in-product help facility that describes the basic GoldSim features, which can be used to supplement this manual. The Help system can be accessed by selecting **Help | Help Topics** from the main GoldSim menu or the Help button (the question mark) on the standard toolbar. Pressing the **Help** button within any of the dialogs also provides access to Help (in a context-sensitive manner).

All of the information in the **GoldSim User's Guide**, the **GoldSim Contaminant Transport Module User's Guide**, and other extension module

user guides (e.g., the **GoldSim Distributed Processing Module User Guide**) is accessible via GoldSim Help. Note, however, that information included in the appendices of the various user guides is not included in the Help system.

## Technical Support, User Resources and Software Upgrades

The GoldSim Technology Group is dedicated to providing complete solutions for our customers. We pride ourselves in providing prompt and extensive support and resources to our users, and are committed to ensuring that each installation of our software is successful and adds value to the customer.

### GoldSim Maintenance Program

When you purchase GoldSim software, you receive one year of Software Maintenance, entitling you to the following:

- Free software upgrades so that you always have the latest version of the GoldSim software.
- Basic Technical Support via email and phone. Basic support covers installation and licensing questions, as well as questions about GoldSim's features and capabilities.

After the first year, if you wish to continue to have access to new versions and technical support, Software Maintenance can be extended each year with payment of an annual fee.

Details regarding the GoldSim Maintenance Program can be found at [www.goldsim.com/Web/Products/BuyGoldSim/Pricing/MaintenanceProgram/](http://www.goldsim.com/Web/Products/BuyGoldSim/Pricing/MaintenanceProgram/).

### Getting Technical Support

Users with active Software Maintenance can submit questions directly to the GoldSim support team. Evaluation users are also welcome to contact us with questions on GoldSim functionality. The **GoldSim Help Center** (<https://goldsim.zendesk.com>) is the primary portal for technical support. You can submit your questions directly from the Help Center. If you register and log in through the Help Center, you will be able check the status and view a history of all of your support requests.

The Help Center also includes:

- The **GoldSim Forum**, where you can you can post questions to the GoldSim community, or just browse existing messages;
- Articles on licensing questions and modeling tips; and
- An archive of past webinars (which demonstrate GoldSim features and capabilities).

Free Basic Technical Support does not include consulting, model troubleshooting or detailed assistance with applying GoldSim to a particular problem. Assistance of this nature is defined as Advanced Technical Support. Users may purchase Advanced Technical Support in pre-paid 10 hour blocks.

Details regarding Advanced Technical Support can be found at [www.goldsim.com/Web/Resources/TechnicalSupport/](http://www.goldsim.com/Web/Resources/TechnicalSupport/).

### Other GoldSim Resources

In addition to the GoldSim Help Center, additional resources are also available. These three resources can be accessed directly from the GoldSim website ([www.goldsim.com](http://www.goldsim.com)):

- A free **Online Training Course** that will provide you with a thorough understanding of the key concepts on which GoldSim is based and all

of the fundamentals required to build complex models of nearly any kind of system.

- The **GoldSim Model Library**, which contains a collection of example models to allow you to see how specific features of GoldSim can be used and/or how GoldSim can be used for specific applications.
- The **GoldSim Blog**, which provides an informal mechanism for GoldSim staff to share their knowledge, point out some of the more advanced (and perhaps overlooked) GoldSim features, share and discuss common mistakes we see in GoldSim applications, discuss interesting applications, and keep you abreast of our plans for further GoldSim developments.

You can stay up to date on the latest GoldSim news through these resources:

- The GoldSim LinkedIn Group, which is primarily used for announcements (e.g., new versions, interesting applications). You can join the Group here: [www.linkedin.com/groups/1798413](http://www.linkedin.com/groups/1798413)
- Periodic email newsletters are sent two to three times per year. To be added to the newsletter list, contact us via the GoldSim Help Center (<https://goldsim.zendesk.com>).



**Note:** When you purchase GoldSim, you are entitled to a free one hour, live web-based training session in which one of our analysts provides an interactive training session via the Internet and telephone. You are strongly encouraged to take advantage of this free training.

---

---

# Chapter 2: Contaminant Transport Module Overview

A poet physicist once calculated how many atoms from Plato's body each of us has appropriated as our own - probably in excess of  $10^{10}$ . Behind the vertigo of the multiple reincarnations and the comforting thought of all the great people each of us has been lies the profound and fundamental principle of the conservation of mass.

Francois M.M. Morel, *Principles of Aquatic Chemistry*

## Chapter Overview

This chapter provides an introduction to and a "quick tour" of the GoldSim Contaminant Transport Module. It presents the basic concepts of how contaminant transport is simulated in GoldSim, provides an overview of the features and capabilities of the program, summarizes the specialized elements associated with the module, and outlines the steps required to build a contaminant transport model for an environmental system.

If you read nothing else in this manual before starting to use the Contaminant Transport Module, it is strongly recommended that you read this chapter, as it will tell you what the module is capable of doing, provide an overview of how to build a contaminant transport model, and direct you to those portions of the manual where you can obtain further information.



**Warning:** This chapter assumes that you are familiar with the basic capabilities of GoldSim. If not, you should refer to the **GoldSim User's Guide**.

---

### In this Chapter

This chapter discusses the following:

- Top-Down Modeling Philosophy
- Modeling Contaminant Transport Using GoldSim: Basic Concepts
- Features and Capabilities of Transport Pathways
- What Does the Contaminant Transport Module Add to the GoldSim User Interface?

- Building a Contaminant Transport Model in GoldSim
- Using Features of the GoldSim Simulation Framework in Contaminant Transport Models
- Where Do I Go From Here?

## Top-Down Modeling Philosophy

Before describing the GoldSim Contaminant Transport Module in detail, it is important to first discuss the underlying philosophy incorporated into its overall design.

In general terms, there are two ways to approach any kind of modeling problem: from the "*bottom-up*", or from the "*top-down*". Although the GoldSim Contaminant Transport Module can be readily used in a "bottom-up" manner, it was specifically designed to facilitate "top-down" modeling.

### What is "Bottom-Up" Modeling?

"Bottom-up" modeling approaches attempt from the outset to acquire data and model the various controlling processes in great detail, and typically make use of complex *process-level models* for the various system components. The emphasis is on understanding and explaining the processes in great detail in order to eventually describe the behavior of the entire system.

While such an approach may seem at first glance to be "scientifically correct", for the following reasons it is generally not the best way to solve real world problems:

1. The level of detail in a model developed from the bottom-up often becomes inconsistent relative to the amount of available information. That is, a model is only as good as its inputs, and if you don't have much information, a detailed model is generally no better than a simple one.
2. It is often difficult to appropriately integrate and capture interdependencies among the various model components in a bottom-up model, since it is often impossible (or computationally impractical) to dynamically couple the various detailed process-level models used for the components of the system. As a result, important interactions in the system are often intentionally or unintentionally ignored in a bottom-up model.
3. It is easy for a bottom-up modeling project to lose sight of the "big picture" (i.e., to "not see the forest for the trees"). As a result, such an approach can be very time-consuming and expensive, with much effort being spent on issues that prove to have little or no impact on the ultimate objective of the project.
4. Finally, and perhaps most importantly, such models tend to be very difficult to understand and explain (and hence be used) outside of the group of people who create them.

### What is "Top-Down" Modeling?

"Top-down" modeling approaches, on the other hand, start from the top (i.e., the ultimate objective of the modeling exercise) and concentrate on the *integration* and coupling of all system components. The controlling processes may initially be represented by approximate high-level (i.e., less detailed or "abstracted") models and parameters. The model can then evolve by adding detail (and reducing uncertainty) for specific components as more is learned about the system. Such an approach can help to keep a project focused on total system performance without getting lost in what may prove to be unnecessary details. Moreover, because a properly designed top-down model tends to be only as

complex as necessary, is well-organized, and is hierarchical, it is generally easier to understand and explain to others.

There are two key points in the application of a top down modeling approach:

1. Top-down models must incorporate an accurate representation of the *model and parameter uncertainty* resulting from the approximations.
2. As opposed to representing all processes with great detail from the outset, details are only added when justified (e.g., if additional data are available, and if simulation results indicate that performance is sensitive to a process that is currently represented in a simplified manner). That is, details are only added to those processes that are identified as being important with respect to system performance and where additional detail will reduce the uncertainty due to model simplifications.

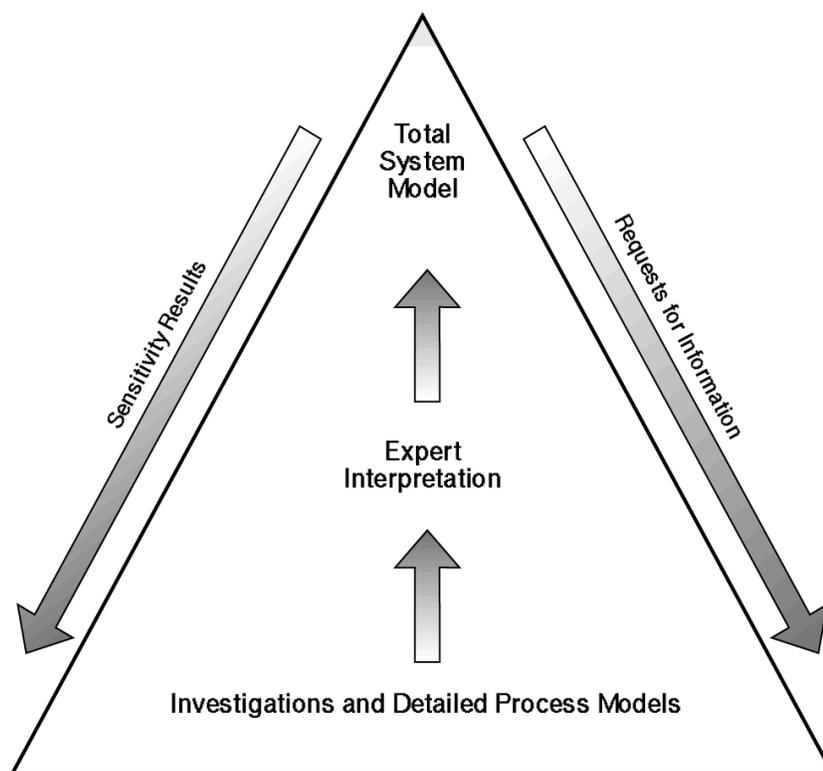
It is important to understand that a top-down model does not have to be “simple”. Whereas a “simple” model might completely *ignore* a key process, a well designed top down model *approximates* the process while explicitly incorporating the resulting uncertainty that is introduced. Hence, in a top-down approach to system simulation, the objective is not to *explain* the detailed behavior of all aspects of the system, but rather to be as comprehensive as possible by integrating the available information in an attempt to *describe* the possible range of system behavior. That is, the focus of a top-down approach is on the ultimate *performance* of the system, as opposed to understanding all the details of the *processes* contributing to that performance.

It is important to reiterate that for the reasons stated previously, the maximum predictive capability does not always lie in the most complex model. In fact, qualified expert judgment may be preferable to using any model at all in some cases (i.e., in cases where either the models or the available data are unreliable or do not represent the actual system). As a simple example, consider the case where one wishes to predict the temperature in Seattle on March 15 of next year. A “high-level” top-down approach to this problem might be to use an almanac to obtain average weather statistics in the month of March, and subjectively assess the degree of variability expected from day to day to obtain a probability distribution for the temperature on that date. A “low-level” bottom-up approach to this problem would be to use a global climate model computer program, and carry out simulations to obtain a probability distribution of the temperature on that date. Clearly, the top-down approach would be just as accurate (if not more accurate) than the bottom-up approach in this case. Although this is an extreme example, it does help to illustrate that complex models are not always technically better than “simple” models, a point often overlooked by scientists and engineers involved in complex modeling efforts.

Although detailed process-level models may not be directly implemented when using a top-down approach, this is not to say that detailed modeling is not required. Quite to the contrary, detailed process-models form the foundation for a top-down model and are always required to some extent in order to generate the appropriate input parameters, and to assess the degree of approximation involved in simplified approaches.

The figure below schematically illustrates the information flow within a top-down modeling approach. Note that information must flow in both directions. At the base of the system are process-level models and field and laboratory experiments. This information (i.e., what processes to include, what processes to ignore, what input values to use, what level of uncertainty to assume) is then assimilated by experts into a form that can be used in a top-down *total system*

*model.* The downward flow of information from the total system model consists of identification of the processes and parameters to which system performance is sensitive, and requests for further information. With time, the total system model can expand down the pyramid as more details are added to it, and the degree of reliance on expert judgment will be reduced.



In summary, our view is that in almost all situations, you should design your models from the top-down, keeping them as simple as possible, and only adding complexity when it is warranted. As will be seen below and in the following chapters, the GoldSim Contaminant Transport Module can certainly be used in a bottom-up manner, and you can readily build very complex models. GoldSim was specifically designed, however, to facilitate top-down modeling, and we strongly encourage you to use the program in this way.

## Modeling Contaminant Transport Using GoldSim: Basic Concepts

The GoldSim Contaminant Transport Module is a *mass transport model*. A mass transport model is a mathematical representation of an actual system (e.g., the subsurface environment near a waste disposal site) which can be used to simulate (and hence predict) the release, transport (movement) and ultimate fate of mass within the system. The "mass" that is typically simulated is that of chemical contaminants that have been accidentally released or intentionally disposed of within the system.

### Contaminant Species

GoldSim allows you to simulate the transport of an unlimited number of species (types of chemical constituents) within an environmental system. The species can undergo complex user-specified chemical reactions as they are transported through the system. The species can be defined to behave independently, or can

be coupled by either being specified as part of a reaction (decay) chain or as isotopes of the same chemical element.



**Note:** Simulation of decay chains (reaction or daughter products) requires the RT Module. The CT Module can simulate decay, but cannot represent reaction products.



**Note:** Although the species in a GoldSim model will typically represent chemicals (man-made or naturally occurring), you can also use GoldSim to model the transport of other types of mass in an environmental system, such as bacteria, viruses or particulate matter such as dust or suspended sediments. You can even use GoldSim to simulate the transport of heat.

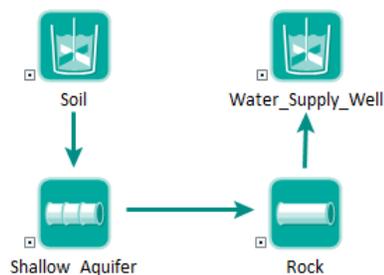
**Read more:** [Creating and Editing Species](#) (page 43); [Simulating Non-Chemical Constituents](#) (page 303).

## Modeling Transport Pathways

The GoldSim Contaminant Transport Module allows you to simulate the transport of mass through an environmental system by providing a number of specialized GoldSim elements. The most important of these is the *transport pathway* (of which there are several types).

Transport pathways represent physical components through which contaminant species can move and/or be stored, such as aquifers, lakes, sediments, surface soil compartments, and the atmosphere. You define the properties of the pathways, such as their geometry and which environmental *media* (e.g., water, soil, air) they contain. All pathways contain one or more environmental media. You define the general properties of each medium (e.g., its density) as well as the properties of each species in each medium (e.g., solubilities and partition coefficients).

You create an environmental system by defining a network of transport pathways, as shown below:



To create such a network, individual pathways are connected via mass flux links. A *mass flux link* defines the mechanisms by which species move between pathways. It represents a vector by species (i.e., it has one item for each species), since the flux will differ for each species being simulated, and has dimensions of mass/time.



**Note:** The Contaminant Transport Module relies heavily on GoldSim's ability to create and manipulate vectors. Therefore, in order to use the module, you must be comfortable with using vectors in GoldSim. If you are not familiar with this capability of GoldSim, refer to "Using Vectors and Matrices" in Chapter 10 of the **GoldSim User's Guide**.

---

Two major types of mass flux links and three special purpose mass flux links can be defined in GoldSim. In an *advective mass flux link*, a quantity of a medium is specified to flow from one pathway to another, carrying dissolved, sorbed, and/or suspended species with it. In a *diffusive mass flux link*, species diffuse between pathways according to a concentration gradient. Three special purpose mass flux links allow you to model processes that cannot be represented as using advection or diffusion. In a *direct transfer mass flux link*, species are moved from one pathway to another based on a user-specified transfer rate. In a *precipitate removal mass flux link*, species present as precipitated mass are moved from one pathway to another based on a specified transfer rate. In a *treatment mass flux link*, species are treated or filtered and are moved to from one pathway to another based on a specified treatment efficiency (a fraction).

---



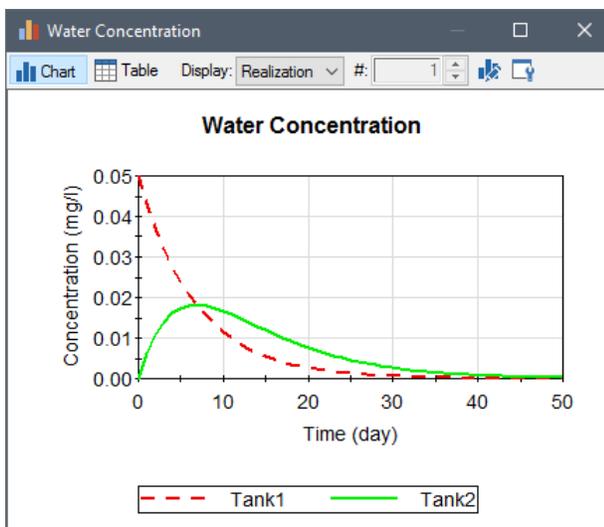
**Note:** The Contaminant Transport Module is a mass transport model, *not* a flow model. That is, it does not directly solve for the movement of media through the environmental system being modeled. Hence, you must directly enter the media flow rates associated with an advective flux link (or provide GoldSim with the equations for computing them).

---

Based on the properties of each pathway, the media in each pathway, the species, and the specified mass flux links, GoldSim computes the temporally varying concentrations in each pathway's media, as well as the mass fluxes between pathways. Hence, the fundamental output of a pathway element is a series of vectors:

- The mass (of each species) in the pathway;
- the concentration (of each species) within each environmental medium in the pathway; and
- the mass flux (of each species) to each of the pathways to which it is connected via mass flux links.

A typical pathway output is shown below:



**Read more:** [Features and Capabilities of Transport Pathways](#) (page 20).

## Modeling Contaminant Sources

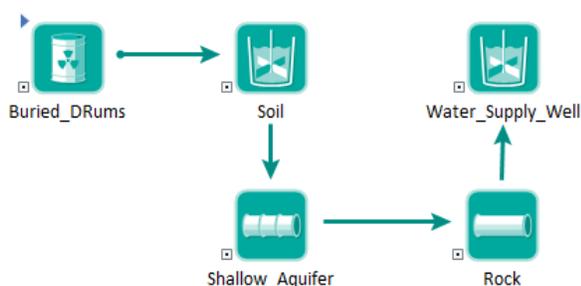


Within GoldSim, there are two ways to introduce mass into the system:

- An initial mass or a rate of addition of mass can be directly specified for one or more pathways in the system; and
- When using the RT Module, the user can define the properties of one or more **sources**, and based on their properties, GoldSim will compute rates of release of mass from the source(s) to specified pathways. (Sources are not available in the CT Module.)

Often, you can use the former method to introduce mass into your model. In many cases, however, direct specification of an initial mass or rate of release at various locations is not possible or appropriate, and explicit modeling of the source is necessary.

Note that the definition of what is meant by a “source” is completely determined by you. A “source” may represent an entire landfill, or a single buried drum; a group of leaking underground tanks or a complex engineered facility. The key point is that the source provides mass input to the pathways that then transport the mass through the system, as illustrated below.



*The Source element named “Buried\_Drums” provides mass input to the Cell pathway named “Soil”.*

The properties of a source which you define consist of 1) the failure rate of any barriers (e.g., drums, boxes) which must fail before the species are released; and 2) the degradation rate of any matrix (e.g., cement, grout) in which the species are bound, which must degrade before the species are released.



**Note:** Sources are only available within the RT Module.

## Modeling Impacts to Receptors



**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4); [Chapter 5: Contaminant Sources](#) (page 259).

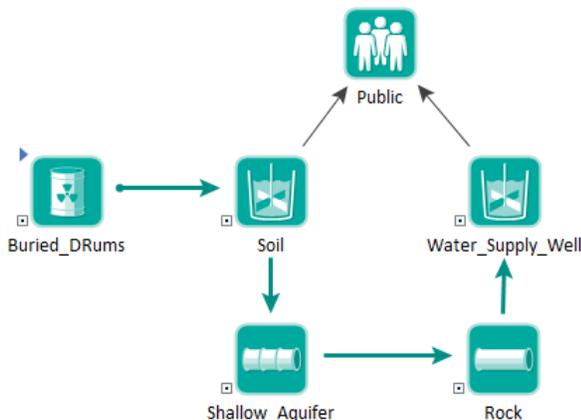
The objective of many contaminant transport studies is to not only compute contaminant concentrations or flux rates at various locations in the environment, but to also compute the impact of these contaminants on specific *receptors* (e.g., humans, wildlife, flora).

This is typically done by multiplying contaminant concentrations in environmental media (e.g., water, soil, air) by user-defined *impact conversion factors*. Impact conversion factors are species- and receptor-specific and have dimensions of impact per unit concentration.

GoldSim allows you to define specific receptors, and associate these with various pathways in your environmental system. The total impact to a receptor is then computed as the sum of the impacts associated with each pathway through which the receptor is exposed to the contaminant (e.g., drinking water from a well, breathing dust in the atmosphere, ingesting soil).

Impacts may be calculated as:

- *ratios* of contaminant concentrations to permissible limits (i.e., hazard quotients);
- health (e.g., cancer) *risks*; or
- radioactive *doses*.



The Receptor named "Public" is exposed to contaminants via the Cell pathways "Water\_Supply\_Well" and "Soil".

**Read more:** [Chapter 6: Receptors](#) (page 289).

## Features and Capabilities of Transport Pathways

Having provided a quick overview of the basic components of the Contaminant Transport Module in the previous section, in this section the computational features of the primary component, the transport pathway, are outlined in somewhat greater detail, as this will provide an indication of the kinds of processes that can be simulated by GoldSim.

GoldSim transport pathways represent physical components through which contaminant species can move (and/or be stored) such as aquifers, lakes, sediments, surface soil compartments, and the atmosphere. In order to represent the wide variety of transport pathways that you may wish to simulate, GoldSim provides five different kinds of pathway elements:

- Cell pathways
- Aquifer pathways
- Pipe pathways
- External pathways
- Network pathways

These pathways can be used interchangeably within a model. Each of these four pathway elements is discussed briefly below.

A Cell pathway is mathematically equivalent to a mixing cell, and can explicitly represent the following processes:

- **Partitioning.** You can assign multiple fluid or solid media (e.g., water, oil, air, rock, soil) to a Cell, and define species partition coefficients between the various media. Contaminant mass is assumed to be instantaneously and completely mixed and equilibrated throughout the Cell, and contaminants are partitioned between the various media based on the partition coefficients and masses/volumes of the various media present.
- **Solubility constraints.** You can assign solubility limits for the contaminants in the fluids (typically water) present in the Cell. The dissolved concentration of the contaminants in the Cell cannot exceed the solubility limit. If you are simulating isotopes of the same element, GoldSim ensures that the sum of the concentrations of all isotopes does not exceed the solubility limit.
- **Mass transport.** You can define the processes and properties controlling the rate at which mass moves between pathways (e.g., from one Cell to another). Both advective and diffusive transport mechanisms can be explicitly represented. You must specify flow rates for advective transport and diffusion coefficients and geometric factors for diffusive transport. You must also specify the media which are being advected (both fluids and solids can be advected), and the media through which diffusion occurs (inter-media diffusion, such as across an air-water interface, can be specified). In addition, solids present in a Cell can be specified to be suspended in the Cell's fluid media, such that the transport of contaminants on suspended particulates (via advection or diffusion) can be explicitly modeled. For special situations, you can also simulate several transfer processes that cannot be described as either advection or diffusion (direct transfer, treatment, and precipitate removal).

When multiple Cells are linked together via advective and diffusive mechanisms, the behavior of the Cell network is mathematically described using a coupled system of differential equations. In effect, a network of Cells is mathematically equivalent to a finite difference network of nodes. GoldSim numerically solves the coupled system of equations to compute the contaminant mass present in each Cell (and the mass fluxes between Cells) as a function of time.

## Cell Pathway Features



## Aquifer Pathway Features



Cells are commonly applied to simulate discrete compartments in an environmental system (such as ponds, lakes, shallow soil compartments, or the atmosphere). In some situations, a series or network of Cells may also be the best way to simulate features such as aquifers and rivers.

**Read more:** [Using Cell Pathways](#) (page 119).

An Aquifer pathway is intended to represent a feature that essentially behaves as a *fluid conduit*. It provides a way to simulate processes such as vertical transport through an unsaturated (vadose) zone, and horizontal transport in aquifers, rivers, channels and pipelines.

Aquifer and Pipe pathways can be used for many of the same purposes. Depending on the system to be simulated, however, one is typically preferred over the other.

**Read more:** [Comparing Pipes and Aquifers](#) (page 89).

Unlike Cell pathways, Aquifer pathways can contain only a single fluid medium. They can, however, contain a solid medium which can impact transport (e.g., by modifying the porosity of the pathway and/or acting to sorb and hence retard species).

An Aquifer pathway actually performs its computations by creating a temporary set of linked Cell elements during the simulation, which are subsequently removed at the end of the simulation. In most cases, there is no need for you to be aware of how this is done, or to view the temporary Cell pathways that are created.

Because Aquifers internally use Cells to carry out their calculations, they can represent most of the same processes that can be represented by a Cell network. In particular, Aquifers can represent the following:

- **Partitioning.** Within each internal Cell contaminants are partitioned between the Reference Fluid and the Infill Medium based on the partition coefficients and masses/volumes of the various media present.
- **Solubility constraints.** You can assign solubility limits for the contaminants in the Reference Fluid (typically water) present in the pathway. The dissolved concentrations of the contaminants in the pathway cannot exceed the solubility limits. If you are simulating isotopes of the same element, GoldSim ensures that the sum of the concentrations of all isotopes does not exceed the solubility limit.
- **Mass transport.** Advective, dispersive and diffusive transport mechanisms are explicitly represented within the pathway (using advective and diffusive mass flux links between the internal Cells).
- **Suspended Solids** can be specified to be present in the Aquifer. These Solids are assumed to be advected and dispersed along the Aquifer. Species which partition onto the suspended Solids are transported with them as they move through the Aquifer.

Because multiple Cells are linked together via advective and diffusive mechanisms, the behavior of the Cell network is mathematically described using a coupled system of differential equations. In effect, the network of Cells created within an Aquifer pathway is mathematically equivalent to a finite difference network. GoldSim numerically solves the coupled system of equations to compute the contaminant mass present in the pathway (and the mass fluxes leaving the pathway) as a function of time.

## Pipe Pathway Features



The geometry of the pathway is defined by specifying a length and a cross-sectional area. Conceptually, the pathway may be straight or curved. It simply represents a stream tube for the advecting medium.

Aquifer pathways are ideal for simulating processes such as vertical transport through an unsaturated (vadose) zone and horizontal transport in aquifers, rivers, channels and pipelines.

**Read more:** [Using Aquifer Pathways](#) (page 174).

A Pipe pathway is intended to represent a feature which essentially behaves as a *fluid conduit*. Mass enters at one end of the conduit, advects through (and disperses within) the conduit, and then exits at the other end of the conduit.

Aquifer and Pipe pathways can be used for many of the same purposes. Depending on the system to be simulated, however, one is typically preferred over the other.

**Read more:** [Comparing Pipes and Aquifers](#) (page 89).

Unlike Cell pathways, Pipe pathways can contain only a single fluid medium. They can, however, contain solid media which can impact transport (e.g., by modifying the porosity of the pathway and/or acting to sorb and hence retard species).

Pipe pathways use a Laplace transform approach to provide analytical solutions to a broad range of advectively-dominated transport problems involving one-dimensional advection, longitudinal dispersion, retardation, decay and ingrowth, and exchanges with immobile storage zones (e.g., matrix diffusion).

Two types of simple contaminant retardation processes can be represented within a Pipe pathway:

- equilibrium partitioning between the fluid in the pathway and a user-specified infill material; and
- equilibrium partitioning between the fluid in the pathway and a user-specified coating material (around the perimeter of the pathway).

In addition to these linear retardation mechanisms mentioned above, Pipe pathways can also represent interchanges with two types of immobile storage zones along the length of the pathway:

- *matrix diffusion zones*, in which the transfer rate into and out of the zone is proportional to the concentration difference and the diffusive properties of the zone; and
- a “*stagnant*” *dispersive zone*, in which the transfer rate into and out of the zone is proportional to the concentration gradient and the flow rate in the pathway.

Finally, suspended Solids (e.g., colloids) can be specified to be present in a Pipe. These Solids are assumed to be advected and dispersed along the Pipe, but are not subject to retardation processes or interactions with storage zones. Species which partition onto the suspended Solids are transported with them as they move through the Pipe.

The geometry of the pathway is defined by specifying a length, a cross-sectional area, and a perimeter. Conceptually, the pathway may be straight or curved. It simply represents a stream tube for the advecting medium.

Pipe pathways may be used for simulating processes such as vertical transport through an unsaturated (vadose) zone, and horizontal transport in aquifers,

rivers, channels and pipelines. They are particularly valuable for simulating transport through fractured rock masses.

**Read more:** [Using Pipe Pathways](#) (page 194).

### External Pathway Features



External pathways provide a mechanism by which external program modules for contaminant transport (e.g., analytical, finite element or finite difference transport models) can be directly integrated into GoldSim. These modules are linked into GoldSim as DLLs (Dynamic Link Libraries) at run time.

You determine the manner in which the External pathway operates on the contaminant mass it receives: the External pathway may be a simple one-dimensional representation, or could be a complex three-dimensional model.

You define the manner in which the External pathway is linked to the rest of the pathway network by specifying the input mass flux links (i.e., the pathway(s) which discharge mass to the External pathway) and the output mass flux links (i.e., the pathway(s) to which the External pathway discharges mass). GoldSim then automatically calls the function representing the External pathway at the appropriate times, passing the appropriate information back and forth between GoldSim and the function.

Integrating external contaminant transport modules into GoldSim requires that you develop a "wrapper" (or "shell") around your existing function, and in most cases, this will require only a limited number of programming modifications.

**Read more:** [Using External Pathways](#) (page 219).

### Network Pathway Features



Network pathways provide a computationally efficient way to simulate large, complex networks of one-dimensional conduits in order to describe contaminant transport through fractured rock systems.

A Network pathway is made up of multiple "pipes". Each pipe has all the features and capabilities of the Pipe pathways discussed above. Hence, Network pathways are effectively large collections of Pipe pathways. The network, however, can be very large (e.g., 100,000 pipes). This allows complex and realistic fracture systems to be simulated.

Network pathways require specification of a *fracture network*, which can be entered by hand, but more likely, would be generated by a discrete fracture network generation and flow simulation code. The fracture network identifies all of the pipes in the network, the manner in which they are connected, and each pipe's geometry and flow rate. In addition, for each pipe, it specifies the *fracture set*, which identifies the transport properties of the pipe (e.g., porous infill material, coating material, properties of matrix diffusion zones, etc.).

GoldSim uses a Laplace transform algorithm to solve complex fracture networks in a very efficient manner. In fact, even large networks (100,000 pipes or more) can be solved relatively quickly.

To facilitate representation of uncertainty in the fracture network connectivity and flow properties, you have the option to define a number of separate fracture networks and instruct GoldSim to randomly select one of these every realization.



**Note:** Network pathways are only available within the RT Module.

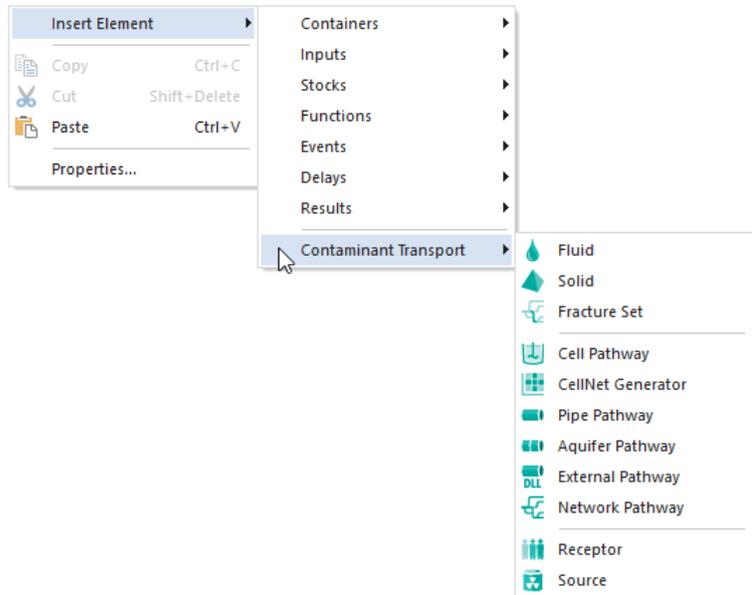
---

**Read more:** [Using Network Pathways](#) (page 232); [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4).

## What Does the Contaminant Transport Module Add to the GoldSim User Interface?

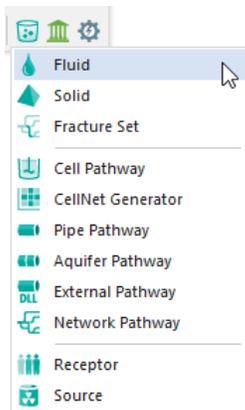
The Contaminant Transport Module is a program extension to the GoldSim simulation framework. As such, it simply adds some additional features to the user interface. The user interface components which the Contaminant Transport Module adds can be summarized as follows:

- An additional item, **Contaminant Transport**, is added to the context-sensitive (right-click) menu in the graphics pane (shown below), to the context-sensitive menu for Containers, and to the **Model Insert** menu on the menu bar:



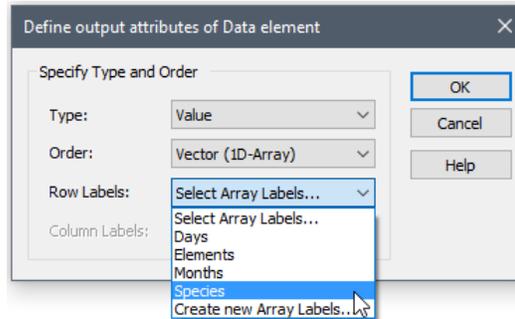
*Note that "Fracture Set", "CellNet Generator", "Network Path", and "Source" only appear if you are using the RT Module. They are not present in the CT Module.*

- Pressing the CT Element button in the Element toolbar provides access to a menu for inserting a CT Module element:



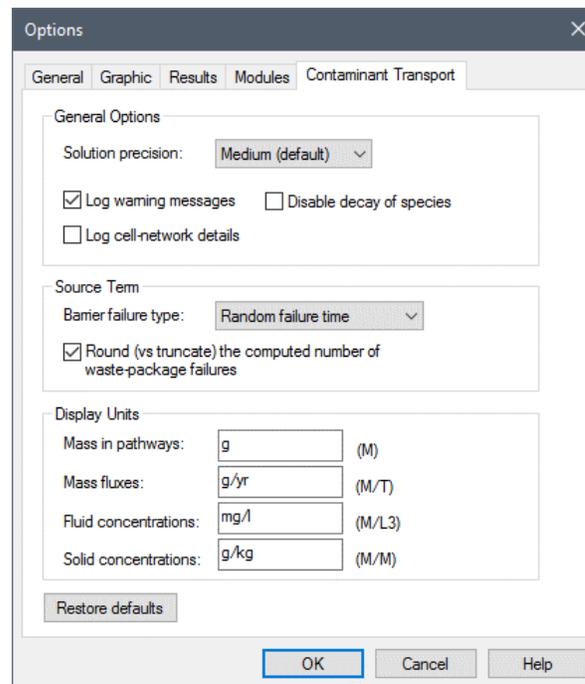
*Note that "Fracture Set", "CellNet Generator", "Network Path", and "Source" only appear if you are using the RT Module. They are not present in the CT Module.*

- When you create a new file, a Material Container is automatically placed in the Model Root. This Container contains a Species element and the Reference Fluid (named Water). These two elements can be moved, but cannot be deleted.
- The *Species* and *Elements* array label sets are added to the drop-down lists available when defining the output attributes for an element:



These sets of array labels are populated when you add species to your model (via a Species element).

- A **Contaminant Transport** tab is added to the Options dialog (accessed via **Model | Options**) for defining options which are specific to the Contaminant Transport Module:



## Building a Contaminant Transport Model in GoldSim

This section briefly outlines the steps required to create a contaminant transport model, and provides a quick tour of each of the GoldSim Contaminant Transport Module elements.

In general, you create a mass transport model of an environmental system within GoldSim in the sequence outlined below:

1. Specify the species to be included in the simulation;
2. Specify the transport and storage media within the environmental system;
3. Specify the transport pathways in the system;
4. Specify the manner in which the transport pathways are inter-connected via mass flux links;
5. Define the contaminant source terms for the system (if any);
6. Define the receptors who may be impacted by contaminants within the system; and
7. Specify the rate and consequences of any disruptive events that may occur.



**Note:** For all but the most simple models, the most important (and time-consuming) tasks in a contaminant transport modeling project are typically the development of a *conceptual model* and the quantification of the inputs for the system you are trying to simulate. Although the quantification of many of the inputs can be delayed until after you have represented the system in a numerical tool such as GoldSim, development of the conceptual model must, for the most part, occur beforehand. Development of a conceptual model and quantification of inputs are discussed further in Appendix A.

---

**Read more:** [Appendix A: Introduction to Environmental Simulation](#) (page 307).

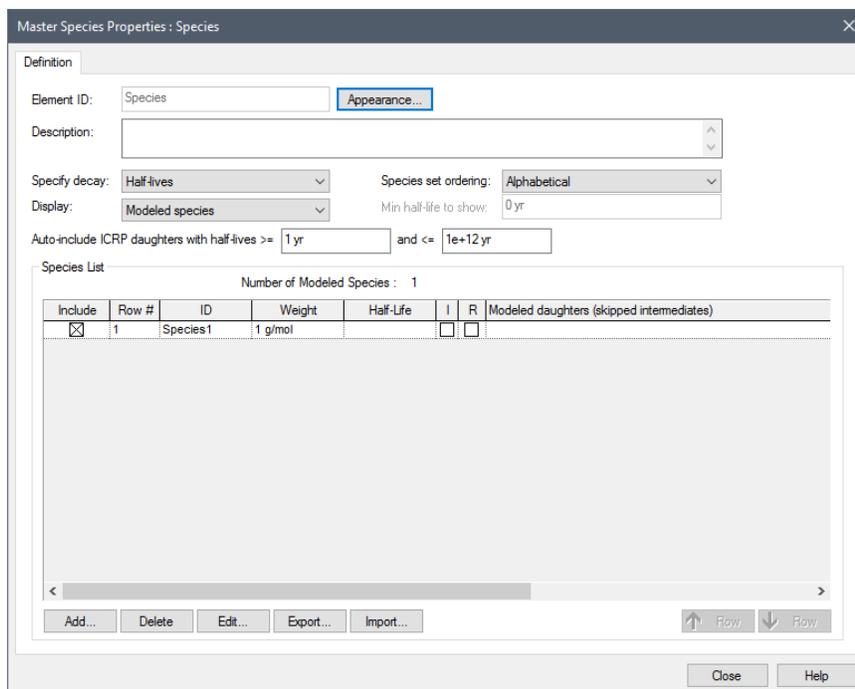
Each of the seven steps listed above is outlined below. The intention of this section is to simply provide a quick overview of these seven steps, and introduce you to each of the Contaminant Transport Module elements. Each of the seven steps is discussed in greater detail in subsequent chapters.

## Defining Species



GoldSim provides a specialized element for defining the contaminant species in a simulation. The *Species* element is located in the Material Container, which is automatically created in the Model Root whenever you create a new file with the Contaminant Transport Module. This element can be moved, but it cannot be deleted.

The Species element is used to add, delete, and edit species. Double-clicking on the Species element brings up the following dialog:



Because the RT Module allows decay chains (daughter products) to be simulated (and to support this, allows you to link to an extensive database of radionuclide decay data), the Species dialog is slightly different depending on whether you are using the RT Module or the CT Module. The screen above is from the RT Module. If you are using the CT Module, some of the fields will not be available.

Species are added (and deleted) using the **Add...** and **Delete...** buttons. (If you are using the RT Module, you also have access to a large database of radionuclide species that can be selected to be included in the model).

**Read more:** [Displaying and Using Species from the ICRP Database](#) (page 47).

Double-clicking on an existing species in the list, or adding a new species displays the Species editing dialog:

The fundamental properties of the species are defined in this window, including the rate at which the species decays (entered as either a half-life or a first-order decay rate), and whether it is part of a decay chain. Although GoldSim requires a first-order decay rate, by making the decay rate a function of the concentration of other species, or of other model parameters (e.g., temperature), nearly any complex reaction can be represented.



**Note:** Decay chains can only be specified in the RT Module.

**Read more:** [Creating and Editing Species](#) (page 43); [Modeling Complex Chemical Reactions](#) (page 299); [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4)

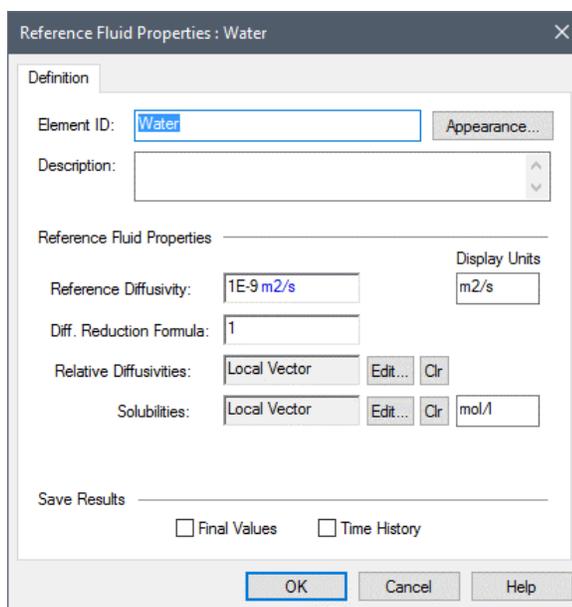
## Defining Media



Before you can define the transport pathways through which the species will be transported, you must first define the environmental media (e.g., water, air, soil) contained in those pathways.

You can define two types of media in GoldSim: **Fluids** and **Solids**. All models contain a **Reference Fluid**. Reference Fluids provide a basis for defining partition coefficients between media for the various species in the model (i.e., the ratio of the species' concentration in the medium to its concentration in the Reference Fluid at equilibrium).

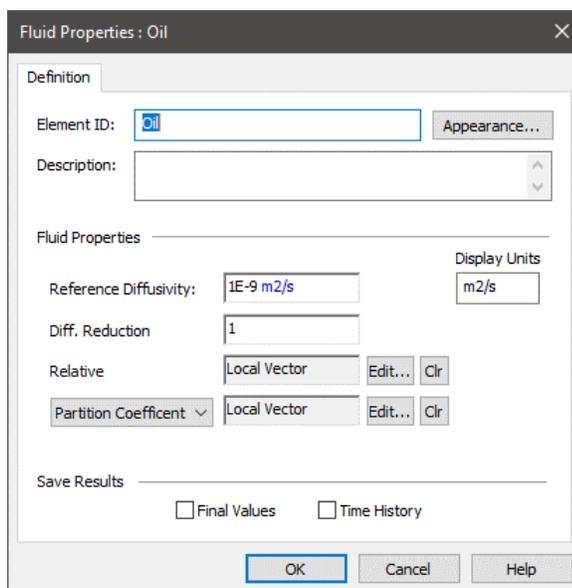
For convenience, the Reference Fluid "Water" is automatically present in the Material Container (which is created in the Model Root whenever you create a new file with the Contaminant Transport Module). The editing dialog for the Reference Fluid looks like this:



The default name for the Reference Fluid is Water, although you can change this if desired. **Relative Diffusivities** and **Solubilities** are vectors, since the property must be defined separately for each species.

You can add additional Fluids and Solids as required (and they can be placed in any Container in the model).

The dialog for other Fluids is similar to that of the Reference Fluid:



When defining a Fluid, you can choose to specify either Solubilities or Partition Coefficients. Partition coefficients are defined relative to the Reference Fluid. Because a partition coefficient is a ratio of concentrations, it is dimensionless for Fluids.

Solid elements require somewhat more information:

The partition coefficients for a Solid are defined relative to the Reference Fluid, and have dimensions of volume divided by mass.

The properties that you specify for Fluids and Solids are perhaps the most important group of inputs in your contaminant transport model. Because each pathway is defined in terms of these media (e.g., the volume of Water or the mass of Sand that exists in a particular pathway), these properties control the way that mass is transported and stored within the pathway network.

Because they represent the fundamental controlling properties of your system, quantifying these inputs in an appropriate manner is essential to producing defensible predictions of contaminant transport. This is discussed further in Appendix A.

**Read more:** [Appendix A: Introduction to Environmental Simulation](#) (page 307); [Creating and Editing Environmental Media](#) (page 64).

## Defining Pathways

After having defined the species and media, you can start to build the network of transport pathways through which the species will be transported.

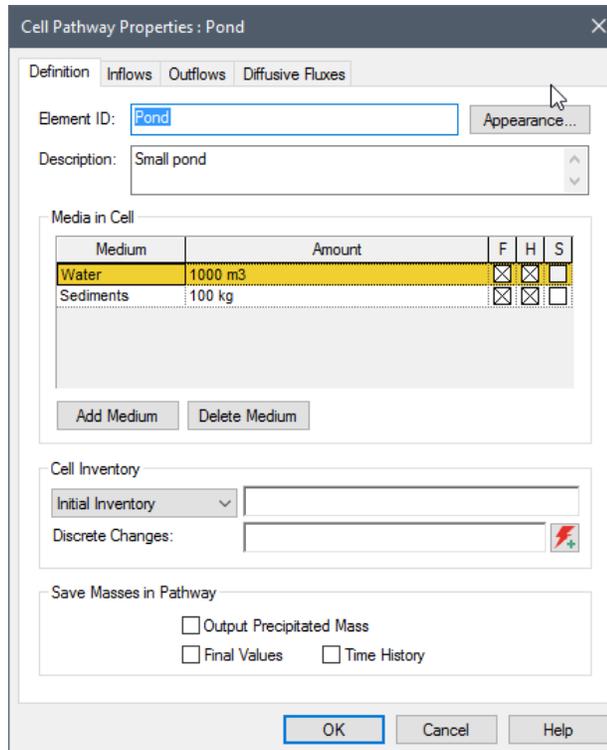
Because there are a variety of transport pathways that you may wish to simulate, GoldSim provides five different pathway elements that you can use interchangeably to build a pathway network. The two most commonly used pathway elements are discussed briefly below.

### Defining Cell Pathways



The most versatile pathway element is the Cell pathway. Cell pathways would typically be applied to simulate discrete, well-mixed environmental compartments such as ponds, lakes, shallow soil compartments, or the atmosphere. In some cases, a series of Cells may also be the best way to simulate features such as aquifers and rivers.

The editing dialog for a Cell pathway looks like this:



The primary input that must be defined for a Cell pathway is the quantity of each medium that is present in the pathway. The Reference Fluid is automatically present in each new Cell. Media are added and deleted using the **Add Medium** and **Delete Medium** buttons. The number of separate media present in a pathway is unlimited, but most Cell pathways will typically include no more than two or three.

The output of a Cell pathway element includes the total mass of each species in the pathway, and the concentration of each species in each medium in the pathway.

**Read more:** [Using Cell Pathways](#) (page 119).

### Defining Aquifer Pathways



Aquifer pathways are intended to represent environmental features that behave as fluid conduits, such as aquifers, rivers, channels and pipelines.

An Aquifer pathway actually performs its computations by creating a temporary set of linked Cell elements during the simulation, which are subsequently removed at the end of the simulation.

The editing dialog looks like this:

The screenshot shows the 'Aquifer Pathway Properties : Aquifer' dialog box. It has three tabs: 'Definition', 'Inflows', and 'Outflows'. The 'Definition' tab is selected. The 'Element ID' is 'Aquifer' and the 'Description' is 'Shallow water supply aquifer'. Under 'Basic Properties', the following values are set: Aquifer Length: 150 m, Aquifer Area: 500 m2, Dispersivity: 15 m, Number of Cells: 10, Infill Medium: Sand, Fluid Saturation: 1, Discrete Changes: (empty), Initial Inventory: (dropdown), Source Zone Length: 0.0 m, and Suspended Solids: Define... There is a checkbox for 'Enable dispersive and diffusive outfluxes to downstream pathway(s)' which is unchecked. At the bottom, there are checkboxes for 'Save Masses and Concentrations in Pathway': Masses: Final Values (checked), Time History (checked); Concentrations: Final Values (checked), Time History (checked). Buttons for 'OK', 'Cancel', and 'Help' are at the bottom right.

The Fluid flowing through the Aquifer pathway is always the Reference Fluid. The geometry of the pathway is defined by specifying an Aquifer Length and an Aquifer Area. You must also define the Number of Cells to be used to discretize the system. Based on this, GoldSim internally creates a series of linked Cell pathways. The specified Infill Medium and Fluid Saturation are used to determine the quantity of media in each Cell. A pathway Dispersivity is also specified. Advective and diffusive flux links are automatically created by GoldSim to appropriately model advection, dispersion and diffusion through the linked Cells.

The output of an Aquifer pathway element consists of the total mass of each species in the pathway, and the concentration of each species in the flowing Reference Fluid exiting the pathway (i.e., in the last Cell).

**Read more:** [Using Aquifer Pathways](#) (page 174).

## Interconnecting Transport Pathways

A mass transport model simulates the movement of species between pathways. Hence, the pathways that you create must be interconnected into a pathway network before you can simulate contaminant transport.

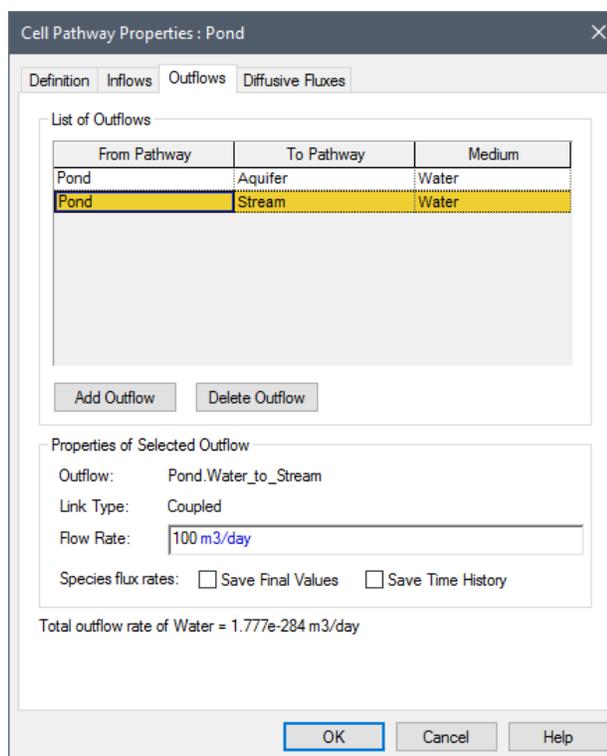
Pathways are connected together into a network by creating *mass flux links* between pathways. Mass flux links control the rate at which each species is transported between pathways. Mass flux links are created from tabs (**Inflows**, **Outflows**, and **Diffusive Fluxes**) in the pathway editing dialogs. There are two primary types of mass flux links: *advective* and *diffusive*, and 3 special purpose mass flux links: *direct transfer*, *precipitate removal*, and *treatment*.

For most applications, mass transfer between pathways can be represented as a combination of advective and diffusive processes. In some specialized cases (e.g., uptake of contaminants by plants, removal due to treatment processes),

however, it may be necessary to utilize one of the three special purpose flux links to properly represent the kinetics of the mass transfer.

Advective mass flux links (as well as the three special purpose mass flux links) are created from the **Inflows** and **Outflows** tabs, which are nearly identical in appearance. The **Outflows** tab is used to create an advective (or special purpose flux link) *from* the current pathway *to* another pathway. The **Inflows** tab is used to create an advective flux link (or special purpose flux link) *to* the current pathway *from* another pathway.

The **Outflows** tab looks like this:

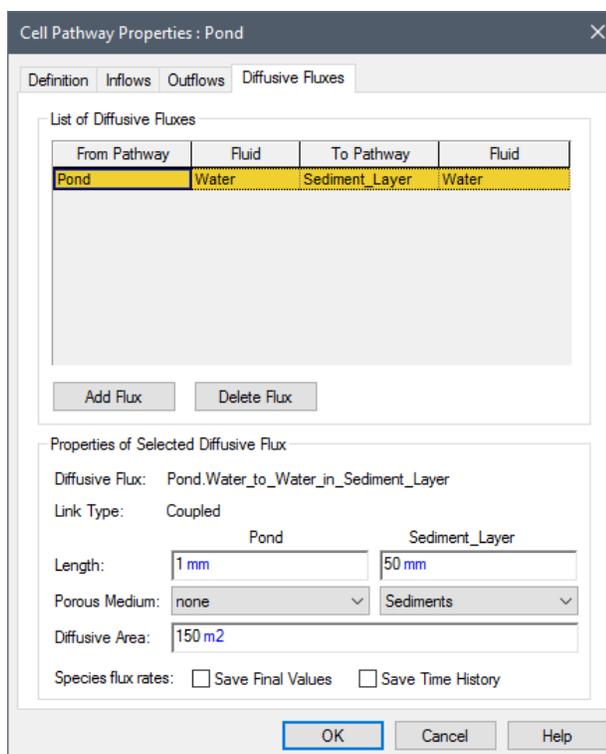


*For each advective mass flux link, you must specify the pathway to which you are connecting, the medium that is flowing, and the flow rate.*

You can create as many advective (and special purpose) outflows (or inflows) as desired in order to build your pathway network. Note that advective and special purpose mass flux links are unidirectional (the flow rate cannot be negative).

Diffusive mass flux links are created from the **Diffusive Fluxes** tab. Whereas advective fluxes can be defined between all types of pathways, all diffusive fluxes must originate in a Cell pathway.

The **Diffusive Fluxes** tab looks like this:



For each diffusive flux link, you must specify the pathway to which you are connecting, the Fluid through which the species are diffusing, and the properties of the diffusive link. The properties of the diffusive link include the geometry of the link and whether the diffusion takes place through a porous medium.

Unlike advective mass flux links, diffusive mass fluxes can be bi-directional. That is, species can be transported in either direction.

Although in most cases, the mass flux between two pathways will be dominated by either advection (e.g., advection in flowing water) or diffusion (e.g., diffusion through stagnant water), in some situations it will be appropriate for pathways to be simultaneously connected by both advective and diffusive links (e.g., advection and diffusion in slowly flowing water).

**Read more:** [Creating Mass Flux Links](#) (page 90).

The assumptions and mathematical details upon which the transport pathway elements are based are described in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

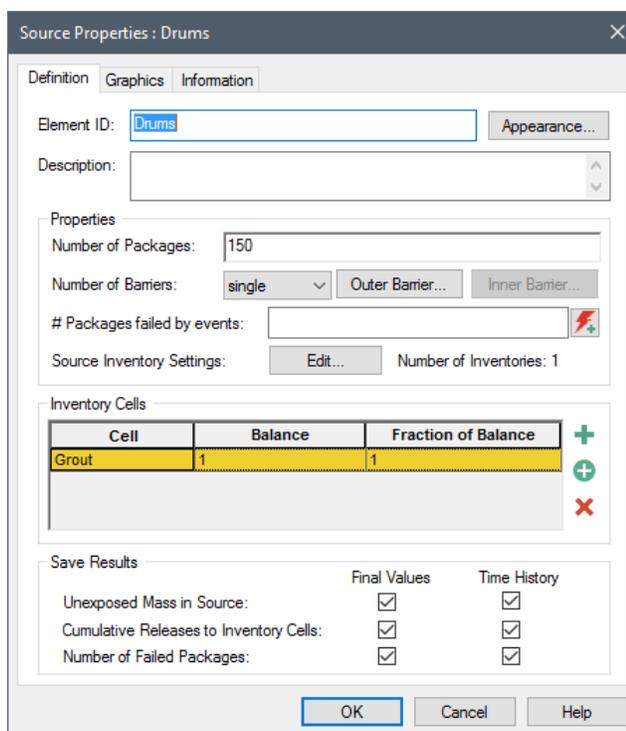
## Defining Sources



One way to specify a source of contamination in a contaminant transport model is to simply specify an initial mass of contaminant or a rate of addition of mass for one or more transport pathways. In many cases, however, it may be necessary to explicitly model a source such that the effect of the barriers (such as drums or boxes) and/or waste matrix (e.g., cement) in which the species are initially contained can be more accurately represented.

This is particularly important when simulating the behavior of proposed or existing waste disposal facilities which have, as part of their design, engineered packages or containers in which the waste is placed prior to disposal.

GoldSim provides a Source element that allows you to accomplish this. The editing dialog for a Source looks like this:



Inputs to a Source element include the rate at which the packages containing the waste fail, the amount of initial mass of each species (the inventory), the location of the inventory (with respect to the barriers), the degradation rate of any matrix material in which the inventory is initially contained, and the pathways to which the mass from the Source will be released.



**Note:** Source elements are only available in the RT Module.

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4).

The outputs from the Source include the amount of mass of each species remaining in the Source, the cumulative amount of mass of each species which has been released, and the number of failed packages.

**Read more:** [Chapter 5: Contaminant Sources](#) (page 259).

The assumptions and mathematical details upon which the Source element is based are described in Appendix E.

**Read more:** [Appendix E: Details of Source Computations](#) (page 399).

The objective of many contaminant transport calculations is to not only compute contaminant concentrations or flux rates at various locations in the environment, but to also compute the impact of these contaminants on specific *receptors* (e.g., humans, wildlife, flora).

Impacts may be calculated as:

- ratios of contaminant concentrations to permissible limits (i.e., hazard quotients);
- health (e.g., cancer) risks; or
- radioactive doses.

## Defining Impacts to Receptors



Impacts such as these are typically computed by multiplying the concentrations in an environmental medium to which the receptor is exposed (e.g., water in a well) by a set of **impact conversion factors**. Impact conversion factors are species- and receptor-specific, and have dimensions of impact per unit concentration.



**Note:** Computing the impact to a receptor always involves carrying out a term-by-term multiplication of a concentration vector and an impact conversion factor vector. As described in "Using Vectors and Matrices" in the **GoldSim User's Guide**, you can carry out a term-by-term multiplication of two vectors using the \* operator.

Within GoldSim, you could compute an impact by using an Expression element to carry out a term-by-term multiplication of the species concentration vector for a particular medium in a pathway by a vector of impact conversion factors. For convenience, the Contaminant Transport Module provides a specialized version of an Expression element (a Receptor element) to facilitate this calculation. The dialog for this element looks like this:

Receptor Properties : Resident

Definition

Element ID:  Appearance...

Description:

Receptor Properties

Impact Type:

Impact:

Output Attributes

Vector by Species      Dimension: L2T-3

Display Units:

Save Results

Final Values     Time History

OK    Cancel    Help

The **Impact Type** determines the dimensions of the impact which is computed. The equation computing the impact is entered directly below the type. The output of this equation must be a vector by species, with the dimensions being consistent with the specified impact type.

Typically, the impact to a receptor will be a sum of several term-by-term vector multiplications, since the receptor is likely to interact with multiple contaminated media (e.g., water in a well, soil, dust).

**Read more:** [Chapter 6: Receptors](#) (page 289).

## Defining Disruptive Events

The final step in creating your contaminant transport model is to define the occurrence and consequence of any disruptive events that may impact your system.

GoldSim provides the ability to model the occurrence and consequences of discrete events (see "Simulating Discrete Events" in the **GoldSim User's Guide**). For example, you could simulate an event such as an earthquake which

has the consequence of instantaneously changing the value of some parameters in the model (e.g., increasing the flow rate in a pathway) when the event occurs.

In addition to changing parameter values, the GoldSim Contaminant Transport Module allows you to use events and consequences to instantaneously move mass from one pathway (or Source) to another pathway, and/or to disrupt packages in a Source in response to an event such as an earthquake or an industrial accident.

**Read more:** [Simulating Discrete Changes to the Mass Inventory in a Cell](#) (page 132); [Disrupting Packages Using Discrete Events](#) (page 281).

## Using Basic GoldSim Features in Contaminant Transport Models

It is important to keep in mind the basic features of the GoldSim simulation framework as you build your contaminant transport model, as these greatly expand the power and flexibility of the tool. Three key of these basic features are highlighted below.

### Utilizing the Basic GoldSim Elements in a Contaminant Transport Model

Nearly all of the inputs to the GoldSim Contaminant Transport Module elements accept links from other GoldSim elements (with compatible data type and dimension). For example, you could define the length of a pathway using an Expression, or the partition coefficient of a species for a particular medium using a Look-Up Table.

If necessary, you can even link an external DLL to your model using GoldSim's External element. This, for example, would allow you to dynamically define the solubilities using a geochemical equilibrium code.

GoldSim's Extrema element is also likely to be useful when carrying out contaminant transport simulations. The Extrema element allows you to compute the highest or lowest value achieved by a particular output over the course of a simulation. For example, you could use an Extrema element to compute the peak concentration in a particular medium in a pathway, or the peak impact to a receptor.

Perhaps the most powerful feature of the GoldSim simulation framework is the ability to describe inputs as probability distributions using Stochastic elements. This is particularly appropriate when simulating contaminant transport through the subsurface, as many of the controlling parameters will necessarily be uncertain. If you describe your inputs using probability distributions, the output of your model will be in the form of probabilistic contaminant transport predictions (e.g., the probability distribution of the peak concentration in a particular pathway).



**Note:** Chapter 4 of the **GoldSim User's Guide**, "Using the GoldSim Elements", describes all of the basic GoldSim elements in detail.

---

### Representing Variability in the Contaminant Transport Module

All real environmental systems are variable to some extent. For example, aquifers are generally heterogeneous with respect to flow and transport properties, chemical conditions vary spatially throughout the environment, and flow rates vary spatially within a stream. Such variability can have a large influence on the behavior of the system, and it is therefore very important to represent this in your model.

## Utilizing GoldSim's Graphical Features in a Contaminant Transport Model

Much of this variability can be directly represented within GoldSim using the basic structure and features of transport pathways and sources. For example, variability in transport pathways can be represented by defining multiple pathways with differing properties, and barrier failure distributions in contaminant sources typically reflect spatial variability in chemical and/or hydrologic conditions.

How would one represent, however, the fact that the decay rate or partition coefficient for a contaminant is spatially variable? In this case, the solution is to define separate Solid, Fluid or Species elements in each location where the properties vary. GoldSim provides some advanced capabilities to facilitate this (localizing Containers and cloning elements). These two features are discussed in detail in Chapter 10 of the **GoldSim User's Guide**.

**Read more:** [Representing Spatial Variability](#) (page 294).

A powerful feature of the GoldSim simulation framework is its ability to incorporate graphics, text, images and hyperlinks into a model. By using these tools, you can create more than just a contaminant transport model of your system - you can create a visual information management system in which the model, the model documentation, and the presentation of results are one and the same.

GoldSim's ability to create top-down, hierarchical models (by using Containers), coupled with these presentation and documentation capabilities allows you to present your model at different (and appropriate) levels of detail to different audiences.



**Note:** These documentation and graphical features are discussed in detail in Chapter 9 of the **GoldSim User's Guide**, "Documenting and Presenting Your Model".

---

## Contaminant Transport Module Online Course

## Where Do I Go from Here?

Using the information presented in this chapter, coupled with the context-sensitive online help (and/or occasional reference to the index or table of contents of this document) will allow you to begin to experiment with the program and build some simple contaminant transport models.

However, it is strongly recommended that instead of “diving in” like this, you first take the online “GoldSim Contaminant Transport Module” training Course. This is the quickest and most effective way to learn how to use the Contaminant Transport Module. The Course will provide you a thorough understanding of the key concepts on which the GoldSim Contaminant Transport Module is based and all of the fundamentals required to build complex models of nearly any kind of system. That is, it does not simply focus on the mechanics of using the Contaminant Transport Module; just as importantly, it explains the fundamental concepts underlying contaminant transport modeling in general.

Because the Course is quite thorough, it will likely take as long as 40 hours to complete. Of course, if you are already familiar with contaminant transport modeling, you may in fact be able to cover the material in considerably less than 40 hours.

The Course is “hands-on”, with many example models, and you can take the Course at your own pace (and the site will remember where you last left off).

## Contaminant Transport Example Models

You can find the Course here:  
<https://www.goldsim.com/Courses/ContaminantTransport/>.

The remaining chapters utilize and discuss examples that are relevant to each chapter. When you install GoldSim, a number of examples are installed with the program. These example model files are mentioned in the text, and provide an excellent way to begin to experiment with GoldSim. Each example is internally documented with comments regarding the way the model was implemented.



**Note:** You can quickly access these files by selecting **File|Open Example...** from the main GoldSim menu. They are all located in a subfolder named Contaminant Transport Examples.



**Note:** Additional (and generally more detailed) example models are available in the Model Library on the GoldSim web site.

---

---

# Chapter 3: Species and Media

Environmental science has learned that chemical behavior in [a] complex assembly of media is not a random process like leaves blowing in the wind. The chemicals behave in accordance with the laws of nature which dictate chemical partitioning tendencies and rates of transport and transformation.

Donald Mackay, *Multimedia Environmental Models: The Fugacity Approach*

## Chapter Overview

This chapter discusses the basic building blocks of an environmental simulation: 1) the species which are to be simulated; and 2) the environmental media in which these species are transported and stored.

Within GoldSim, these are collectively referred to as *materials*. GoldSim provides three specialized material elements: Species, Fluid and Solid. Specification of these material elements is the first step in representing an environmental system within GoldSim.

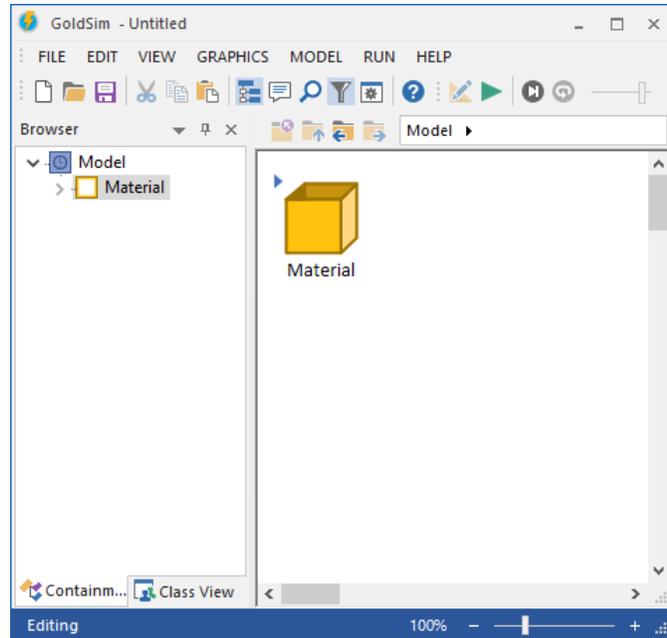
### In this Chapter

This chapter discusses the following:

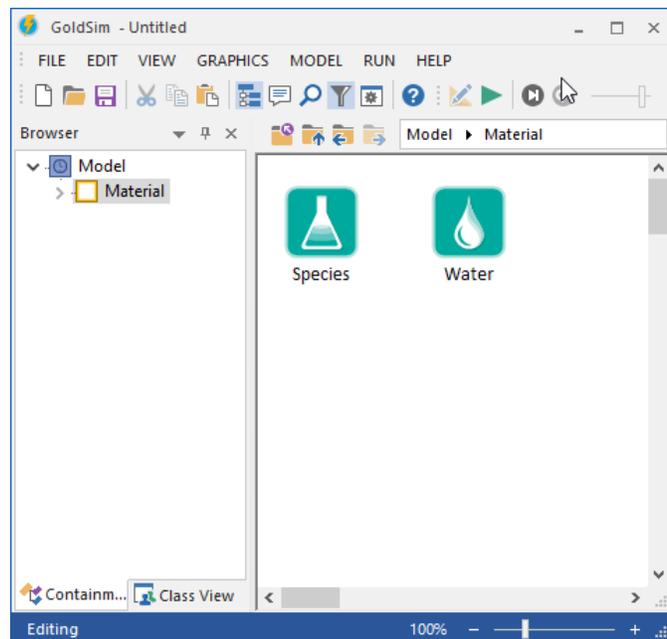
- The Material Container
- Creating and Editing Species
- Creating and Editing Environmental Media
- Copying Material Elements Between GoldSim Model Files

## The Material Container

Whenever you create a new file in GoldSim while the Contaminant Transport Module is enabled (or if you enable the Contaminant Transport Module in an existing file), you will find a Container named "Material" in the Model Root.



This Container contains two elements: the Species element, and the Reference Fluid (named "Water"):



This Container is created only for your convenience. If you want to, you can move these elements out of the Material Container to some other location, and you could then delete the Container. You can also rename the Reference Fluid "Water" to something else (e.g., Blood, Air). Note, however, that GoldSim will not allow you to delete either of these elements.

## Creating and Editing Species



The first step in building a contaminant transport model is to define the species that you wish to simulate. GoldSim allows you to simulate the transport of an unlimited number of species within an environmental system. The species can undergo complex user-specified chemical reactions as they are transported through the system. The species can be defined to behave independently, or can be coupled by either being specified as part of a reaction (or decay) chain or as isotopes of the same chemical element.



**Note:** The RT Module allows decay chains (daughter products) to be simulated (one species can be specified to transform into one or more others). The CT Module allows you to specify decay rates, but you cannot specify reaction (daughter) products.

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4)



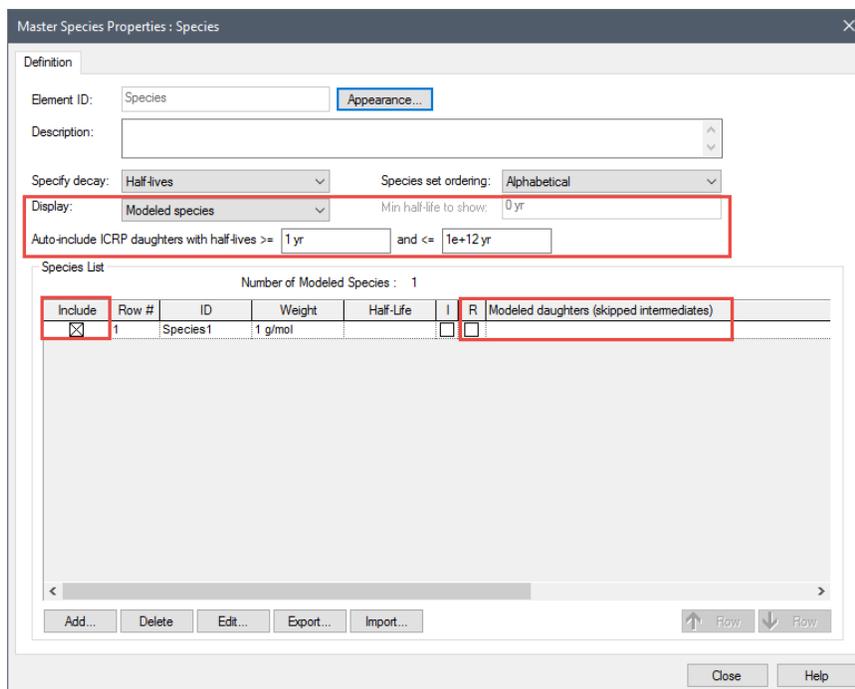
**Note:** Although the species in a GoldSim model will typically represent chemicals (man-made or naturally occurring), you can also use GoldSim to model the transport of other types of mass in an environmental system, such as bacteria, viruses or particulate matter (e.g., dust or suspended sediments). You can even use GoldSim to simulate heat transport.

**Read more:** [Simulating Non-Chemical Constituents](#) (page 303).

Species are defined in a GoldSim model using the Species element. The Species element is originally located in the Material Container when you create a new model with the Contaminant Transport Module. You can move the Species element to a different location, but you cannot delete it.

If you double-click on the Species element, the Species dialog is displayed.

Because the RT Module allows decay chains (daughter products) to be simulated (and to support this, allows you to link to an extensive database of radionuclide decay data), the Species dialog is slightly different depending on whether you are using the RT Module or the CT Module:



The outlined fields (*Display, Min half-life to show, Auto-include ICRP daughters, Include, R and Modeled daughters*) are only available when using the RT Module.

You can enter a **Description** for the species set in the first field. The **Appearance** button accesses a dialog for modifying the appearance of the Species element in the graphics pane.

The dialog displays a list of all the species in the model. By default, a single species called Species1 (which you can rename) exists when you create a new model.

The properties of the species are also displayed. Note, however, that the table of properties cannot be edited directly in the Species dialog. Species properties are edited by double-clicking on a species in the list, or selecting a species and pressing the **Edit...** button.



**Note:** There is one exception to this rule: if you are using the RT Module, the **Include** column is editable under some circumstances. In particular, within the RT Module (but not the CT Module), GoldSim provides an option to utilize a large built-in database of radionuclide decay data (decay rates and daughter products). The **Include** column is used to define which species from the database are used.

**Read more:** [Displaying and Using Species from the ICRP Database](#) (page 47).

## Adding a New Species

To add a new “user-defined” species:

1. Double-click on the Species element in the graphics pane or the browser to access the Species editing dialog.
2. Double-click on the first species (to edit the default species in the list) or press the **Add...** button to add a species and access the Species definition dialog:

3. Enter the **Species ID** and description. The **Species ID** will default to SpeciesN (where N is the number of species defined). You can rename the species. The name must start with a letter, can only contain letters and numbers, and cannot contain any spaces.
4. Define the properties of the species.

**Read more:** [Defining Species Properties](#) (page 52).

You can move through the existing species that you have defined by using the **Previous** and **Next** buttons at the top of the Species definition dialog. If daughters are defined, you can jump directly to those daughters by clicking on the label (e.g., Daughter-1).



**Note:** Some of these fields (Daughter, Stoichiometry and Radioactive) are only available if you are using the RT Module. They are not available in the CT Module.

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4)

Note that within the RT Module (but not the CT Module), GoldSim provides an option to utilize a large built-in database of radionuclide decay data (species, decay rates and daughter products). In particular, you can select from a large set of built-in species instead of manually adding “user-defined” species. If you are using the RT Module but *do not* wish to access species from this database (and just want to add “user-defined” species yourself), simply make sure that the **Display** field in the Species dialog remains set to the default (“Modeled species”).

If you do choose to use the database of species, GoldSim will prevent the name of a “user-defined” species that you add from conflicting with the name of a species included in the database.

**Read more:** [Displaying and Using Species from the ICRP Database](#) (page 47).



**Note:** You can also import species data from a spreadsheet.

**Read more:** [Importing and Exporting Species Data from/to a Spreadsheet](#) (page 58).

## Editing an Existing Species

To edit an existing species:

1. Double-click on the Species element in the graphics pane or the browser to access the Species editing dialog.
2. Double-click on an existing species, or select a species and press the **Edit...** button to access the species definition dialog.
3. Edit the properties of the species.

**Read more:** [Defining Species Properties](#) (page 52).



**Note:** You view, but cannot edit species that are included in the list from the ICRP Database provided by GoldSim within the RT Module.

**Read more:** [Displaying and Using Species from the ICRP Database](#) (page 47).



**Note:** You can also import species data from a spreadsheet.

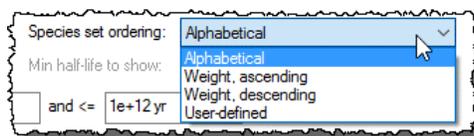
**Read more:** [Importing and Exporting Species Data from/to a Spreadsheet](#) (page 58).

## Reordering Species

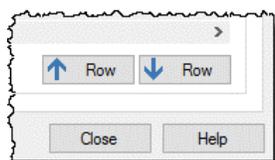
Species are added to the species list shown in the Species dialog in the order that they are created. This is also the default order that they appear in the *species array label set*. (The order that they appear in the species array label set is indicated by the **Row #**). In some situations, however, you may want to change the order in which the species appear in the species array label set.

**Read more:** [The Species and Elements Array Label Sets](#) (page 57).

You can reorder the species via the **Species set ordering** drop-list:



As can be seen, this allows you to sort the species alphabetically or by Molecular Weight. The final option in this list, “User-defined”, allows you to manually move items up and down the list. If this option is selected, the Row Up and Down buttons at the bottom of the page become active:



Selecting a row and pressing one of these buttons moves the species up or down in the list.



**Note:** If you reorder the species, any existing elements using the species array label set will automatically be re-sorted to the new sequence.

---

Note that changing the set order does not actually change how the species are displayed in the Species dialog. It simply changes the **Row #** (and hence the order that the species appear in the species array label set).

By default, when you open the Species dialog, the species will always be displayed alphabetically. You can, however, change how they are displayed in the dialog. You do so by clicking on the column headers. For example, clicking on the **ID** column header sorts the species alphabetically (in ascending order). Clicking it again sorts in descending order. It is important to note, however, that sorting the species by clicking on the column headers in this way does not actually reorder the species in terms of the order of items in the species array label set. It is simply for display purposes while you are in the Species dialog. The **Row #** indicates the actual order of items used in the species array label set, and this can only be changed via the **Species set ordering** drop-list.

While viewing the species, you can also quickly jump to a particular row by placing your cursor in a column and typing the first letter (or number) of a search string. GoldSim will jump to the first corresponding row that it finds.



**Note:** Although you can reorder the species array label set as described above, the elements array label set is always alphabetical.

---

## Displaying and Using Species from the ICRP Database

Within the RT Module (but not the CT Module), GoldSim provides an option to utilize a large built-in database of nuclide decay data (species, decay rates and daughter products). In particular, the feature allows you to view over 1200 nuclides (including both stable and radioactive species) and to selectively include some of these species in your simulation.

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4)

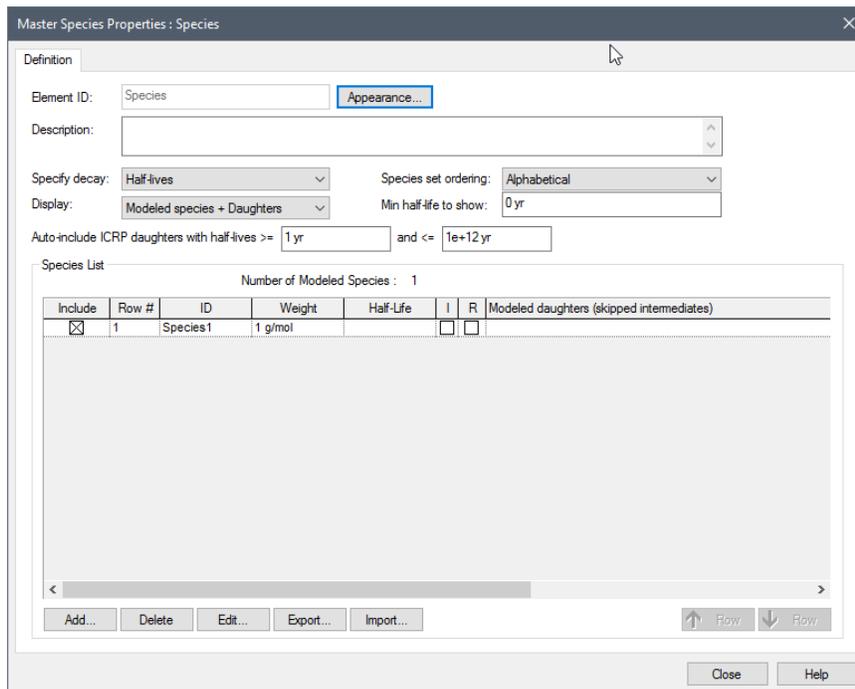
The following should be noted regarding the data used by GoldSim:

- The data is based on the International Commission for Radiation Protection (ICRP)'s Publication 107 (data table ICRP107.NDX). This reference can be viewed here: [http://www.icrp.org/publication.asp?id=ICRP Publication 107](http://www.icrp.org/publication.asp?id=ICRP%20Publication%20107))
- The ICRP table of nuclides contains a list of nuclides with up to three daughters each, along with daughter stoichiometry (i.e., decay branching fractions) and atomic weights.
- The GoldSim implementation uses an updated data set provided by Dr. Keith Eckerman of Oak Ridge National Laboratory in February 2012. This data set corrected minor errors in the atomic weights of some isotopes.
- In some cases where nuclide decays into multiple daughter products, the sum of the ICRP data set's daughter stoichiometry factor is slightly greater than 1.0 due to roundoff. In these cases, GoldSim reduces the

stoichiometry factor for the commonest daughter so the sum of all stoichiometry factors equals 1.0.

- There are some instances where daughter products are not fully specified in the ICRP data set. This is the case for some heavy nuclides (e.g., isotopes of Cf and Cm) that are subject to spontaneous fission, and for some fractional daughters of other nuclides.
- The stable elements included in the data set use the average atomic weight for the naturally-occurring isotopes of the element. This implies that the product of the last decay in a given chain joins the ‘pool’ of naturally-occurring isotopes of the final element.

Within the RT Module, when you open the Species dialog for the first time, it looks like this:



The **Display** field provides access to the full ICRP database. This drop list provides three options:

- **Modeled species** (the default): Displays only those species for which the **Include** box is checked.
- **Modeled species + Daughters**: Displays only those species for which the **Include** box is checked *and* all of their progeny.
- **All species**: Displays all species.



**Note:** If you are using the RT Module but *do not* wish to access species from the ICRP database (and just want to add ‘user-defined’ species yourself), simply make sure that the **Display** field remains set to the default (“Modeled species”).

By default, Display is set to “Modeled species” and a single “user-defined” species (Species1) is listed (and the **Include** box is checked).



**Note:** The **Include** box is always checked (and cannot be cleared) for any “user-defined” species (the default species initially present in all new models, and any additional species added via the **Add** button).

**Read more:** [Adding a New Species](#) (page 44).

To utilize the ICRP database, you will typically initially select “All species”. When you do so, the **Min half-life to show** field becomes available. GoldSim will then display all species from the database (and any custom species you have added manually) whose half-life is greater than that specified or whose **Include** box is checked. That is, GoldSim will exclude from display species which are not **Included** and whose half-life is less than the specified value.

Although GoldSim will display a large number of species when you select “All species”, it is important to understand that this does not mean that they will all be included in your model. The **Include** checkbox is what defines the species to be modeled. That is, only species for which the **Include** box is checked are included in the model. Checking the **Include** box for any species includes it in the model, and clearing the box excludes it from the model.

The final column of the Species element, **Modeled daughters (skipped intermediates)**, indicates which daughters are included in the simulation (and which are excluded), and this is important information to note. If a daughter (or other descendant) of the species is included, it is listed without parentheses. If it is not included, it is listed surrounded by parentheses.

Although the ICRP database includes a very large number of species, any particular model will only use a small subset of these. The subset you select to use will likely be a function of the inventory present, the length of the simulation, and the time scale of the processes being simulated. In most cases, the half-lives of the various species (and their daughters) will play a key role in determining which species are to be included in the model. To facilitate this, GoldSim provides an option to **Auto-include ICRP daughters** within a specified range of half-lives.

To illustrate how the various options can be used, it is most instructive to outline the steps that you will typically take to create your modeled species list using the ICRP database:

1. Select “All species” from the **Display** field.
2. Depending on the time frame of your simulation and the time scale of the processes being simulated, you may then want to specify a **Min half-life to show** in order to hide species with very short half-lives that you know you will not explicitly include in your simulation.
3. In most cases, you will have a list of key species you know must be included in the simulation (e.g., for a disposal facility, species you know will be in the disposal inventory). You should check the **Include** box for each species. Note that you need not consider the daughters for these key species yet. As will be seen in the next step, GoldSim provides a method for automatically including these.



**Note:** GoldSim provides some tools to facilitate finding and selecting species for inclusion. In particular, in any column in the Species dialog, clicking on it sorts it (in ascending order). Clicking it again sorts it in descending order. Clicking a column and then typing in a key combination takes you immediately to that row (e.g., typing Th would take you to the first Thorium isotope in the list).

- If you now select “Modeled species + daughters” from the **Display** list, GoldSim will show only the key species that you have manually included, as well as all of the daughters (in fact, the full chain of descendants) of the key species. You will note that the **Include** box for some of these daughters will be selected and grayed out:

Specify decay: Half-lives      Species set ordering: Alphabetical  
 Display: Modeled species + Daughters      Min half-life to show: 0 yr  
 Auto-include ICRP daughters with half-lives >= 1 yr and <= 1e+12 yr

Species List      Number of Modeled Species : 5

Include	Row #	ID	Weight	Half-Life	I	R	Modeled daughters (skipped intermediates)
<input checked="" type="checkbox"/>	1	Pb-210	209.984 g/mol	22.2 yr	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	(Bi-210, Po-210, Pb, Hg-206, Tl-206)
<input type="checkbox"/>		Pb-214	214 g/mol	26.8 min	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Pb-210 (Bi-214, Po-214, Tl-210)
<input type="checkbox"/>		Po-210	209.983 g/mol	138.38 day	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	(Pb)
<input type="checkbox"/>		Po-214	213.995 g/mol	0.0001643 sec	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Pb-210
<input type="checkbox"/>		Po-218	218.009 g/mol	3.1 min	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Pb-210 (At-218, Rn-218, Pb-214, Bi-214, Po-214, Tl-210)
<input checked="" type="checkbox"/>	2	Ra-226	226.025 g/mol	1600 yr	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Pb-210 (Rn-222, At-218, Po-218, Rn-218, Pb-214, Bi-214, Po-214, Tl-210)
<input type="checkbox"/>		Rn-218	218.006 g/mol	0.035 sec	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Pb-210 (Po-214)
<input type="checkbox"/>		Rn-222	222.018 g/mol	3.8235 day	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Pb-210 (At-218, Po-218, Rn-218, Pb-214, Bi-214, Po-214, Tl-210)
<input checked="" type="checkbox"/>	3	Th-230	230.033 g/mol	75380 yr	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Ra-226
<input type="checkbox"/>		Th-234	234.044 g/mol	24.1 day	<input type="checkbox"/>	<input checked="" type="checkbox"/>	U-234 (Pa-234, Pa-234m)
<input type="checkbox"/>		Tl-206	205.976 g/mol	4.2 min	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	(Pb)
<input type="checkbox"/>		Tl-210	209.99 g/mol	1.3 min	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Pb-210
<input checked="" type="checkbox"/>	4	U-234	234.041 g/mol	2.455e+05 yr	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Th-230
<input checked="" type="checkbox"/>	5	U-238	238.051 g/mol	4.468e+09 yr	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	U-234 (Th-234, Pa-234, Pa-234m)

Note that included species are highlighted in green.

In this example, U-238 has been manually included (the **Include** box has an X). As a result, 4 other nuclides (which are descendants of U-238) have been *auto-included* (and their **Include** boxes are marked as gray). Th-234 (and a number of other nuclides) are listed, but excluded (i.e., the **Include** box is cleared).

The reason for these selections can be explained by the options selected directly above. Since **Display** is set to “Modeled species + daughters”, the daughters of U-238 (and any other manually selected species) are shown in the list. Because **Min half-life to show** is set to 0, none of the daughters are hidden; even very short-lived daughters (such as Th-234) are shown. Finally, because the range for **Auto-include ICRP daughters** is set from 1 yr to 1e+12 years, only daughters with half-lives in that range are *auto-included*.

Hence, auto-inclusion provides a quick and convenient way to include important daughters in the model without having to do so manually.



**Note:** You cannot exclude (clear the **Include** box) for an auto-included species. It is always included, unless the parent that caused it to be auto-included is manually excluded).

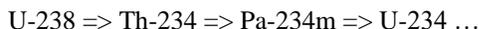
- Based on your auto-inclusion settings, some daughters may still be excluded. You may want to examine these to determine if you would like to include them for a special reason. For example, stable species at the end of the chain will not be auto-included, and you may want to

include these if you think they may be present in significant quantities. Also, you may want to include short-lived species (e.g., Rn-222) that have special transport properties (e.g., they are volatile).

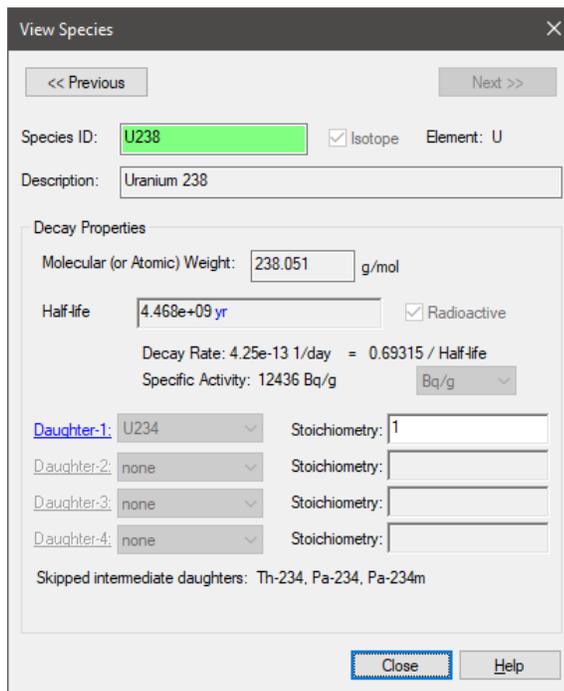
6. All new models initially have a “user-defined” species called Species1. You cannot delete this until you have selected other species to be included (there must always be at least one species). If you have not already done so, you should delete this (by selecting the row and pressing the **Delete** button).
7. To simplify the display, you may want to set the **Display** setting to “Modeled species” such that only the species included in the simulation are shown.
8. You may want to set the **Species set ordering** to define the order of species in the Species array label set.

**Read more:** [Reordering Species](#) (page 46).

It is important to understand what it means to exclude a daughter in a chain. When we do so, the parents of those species “skip over” them and proceed to daughters that have been included. To understand this, consider the U-238 decay chain. The first part of the chain actually looks like this:



However, Th-234 and Pa-234m have short half-lives (less than 1 yr), so if we exclude those two species, GoldSim “skips” them in the decay chain such that U-238 is assumed to decay directly to U-234:



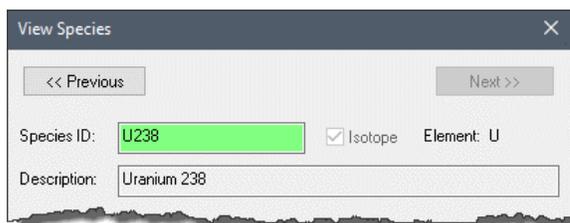
Several additional points should be noted regarding the use of ICRP species:

- Although the ICRP species are shown (in the ID column) with a hyphen separating the element name from the mass number, within the corresponding Species array label set, the hyphen is eliminated (hence, U-238 becomes U238 in the species array label set).

- GoldSim will not let you create a “user-defined” species whose name conflicts with an included species from the ICRP database. Hence, if you try to create a “user-defined” species called U238 and the ICRP species U-238 is marked as included, GoldSim will not let you create the species. Similarly, if a “user-defined” species named U238 already exists, you will not be able to mark the ICRP species U-238 as included.

**Read more:** [Adding a New Species](#) (page 44).

- You cannot edit the properties of the ICRP species. If you click on them in the Species dialog, a dialog for that species will be displayed, but none of the properties can be edited. The **Species ID** of an ICRP species is highlighted in green:



- GoldSim provides the ability to export your species list and subsequently import it (e.g., into another model). If you export a list of ICRP species, when they are subsequently imported, they are always treated as “user-defined” species.

**Read more:** [Importing and Exporting Species Data from/to a Spreadsheet](#) (page 58).

## Removing Species

To delete a “user-defined” species, simply select the appropriate row in the Species dialog and press **Delete**.

If you are using the RT Module, and choose to access the ICRP database of species data, when you do so, you will note that you cannot delete species from the built-in database. You can, however, exclude them from the model (via the **Include** checkbox).

**Read more:** [Displaying and Using Species from the ICRP Database](#) (page 47).

## Defining Species Properties

The properties that you must define for a species in the Species definition dialog are primarily associated with the manner in which the species decays (reacts) as it is transported through the environmental system. Other species properties (e.g., partition coefficients, diffusivities and solubilities) are media-specific and are defined within the Fluid and Solid elements.



**Note:** You view, but cannot edit species that are included in the list from the ICRP Database provided by GoldSim within the RT Module.

**Read more:** [Displaying and Using Species from the ICRP Database](#) (page 47).

## Defining Species Decay Properties

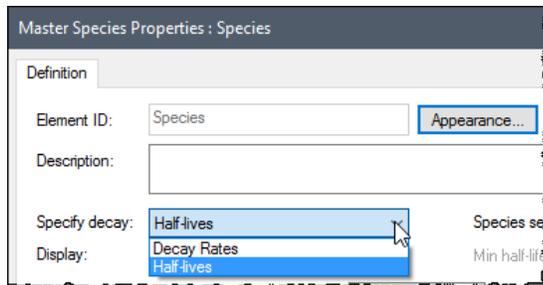
GoldSim allows you to specify that a species decays as it is transported through the system. When a species decays, it can either disappear from the system (i.e., remove mass from the system), or (if you have the RT Module) it can be transformed into up to four reaction products (referred to as *daughters*).



**Note:** You can only edit “user-defined” species that you have manually added to the species list. You view, but cannot edit properties for species that are included in the list from the ICRP Database provided by GoldSim within the RT Module.

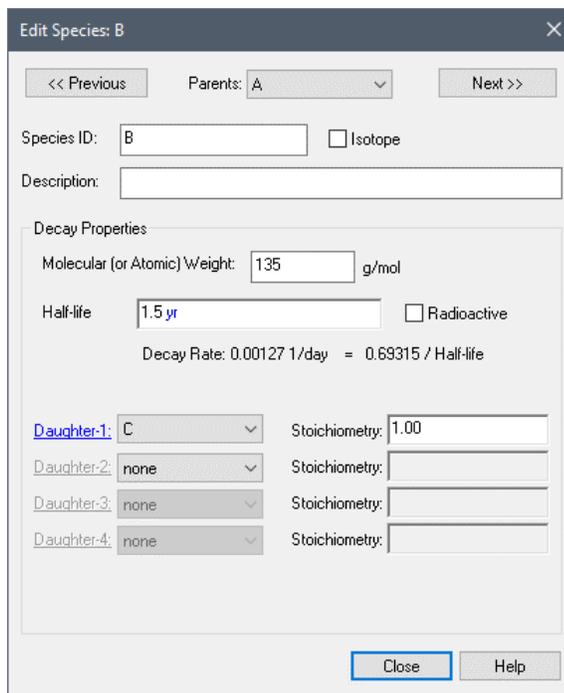
**Read more:** [Displaying and Using Species from the ICRP Database](#) (page 47).

Decay can be defined in terms of a half-life or a first-order decay rate. All species must be defined in the same manner. The manner in which decay is specified is selected on the main species dialog:



By default, decay is defined using half-lives.

The manner in which a species decays is described in terms of the **Half-life** (or **Decay Rate**), the **Molecular (or Atomic) Weight**, the **Daughters**, and the **Stoichiometry**.



**Half-life:** If decay is specified using half-lives, you must enter a half-life for each species (assuming first-order decay). It must have units of time. Note, however, that by making the half-life a function of the concentration of other species, or of other model parameters (e.g., temperature), nearly any complex reaction can be represented. The decay rate of each species is computed as  $\ln(2)/\text{Half-life}$ . The decay rate is displayed directly below the

field using the Time Display Units specified in the Simulation Setting dialog.



**Note:** By default, half-lives for new species default to zero. GoldSim interprets a zero half-life as meaning there is no decay (as opposed to assuming the species decays instantaneously).

**Decay Rate:** If decay is specified using decay rates, you must enter a first-order decay rate for each species. It must have units of inverse time. Note, however, that by making the decay rate a function of the concentration of other species, or of other model parameters (e.g., temperature), nearly any complex reaction can be represented. The half-life of a species with a first-order decay rate is computed as  $\ln(2)/\text{Decay Rate}$ . The half-life is displayed directly below the field using the Time Display Units specified in the Simulation Setting dialog.

**Read more:** [Modeling Complex Chemical Reactions](#) (page 299).

**Molecular (or Atomic) Weight:** This is the molecular or atomic weight of the species. If solubilities are defined based on moles, it is used to convert those to mass based values. When using the RT Module, it is also used to compute the mass of reactants produced based on the stoichiometry which is specified and is required in order to compute the specific activity of radioactive species. Note that this must be entered as a number (it does not accept links).

**Read more:** [Reference Fluid Properties](#) (page 65).

**Daughter-1 through Daughter-4:** These are the decay (reaction) products for the species. You can specify up to four daughters. The drop-down list includes all of the other species in the model. The default is "none". These fields are not available (grayed out) in the CT Module.

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4).

**Stoichiometry:** This is the stoichiometric (molar) ratio, and must be specified for each daughter. It defines the number of moles of daughter produced for each mole of the species which decays. For example, if species A decayed to daughters B and C according to the following reaction:



then the stoichiometry for B would be 0.67 (2/3) and the stoichiometry for C would be 1.67 (5/3). These fields are not available (grayed out) in the CT Module.

You can move through the existing species by using the **Previous** and **Next** buttons at the top of the Species definition dialog. If daughters are defined, you can jump directly to those daughters by clicking on the label (e.g., Daughter-1). Similarly, if the species has a parent, you can jump directly to a parent by clicking on the label at the top of the page.

Mathematically, if A decays to B, GoldSim computes the rate of change of mass (at a particular location) as follows:

$$dM_A/dt = - M_A D_A$$

$$dM_B/dt = M_A D_A R_{BA} W_B / W_A$$

### How GoldSim Simulates Decay

where:

$M_A$  = the mass of species A (mass);  
 $dM_A/dt$  = the rate of change of species A (mass/time);  
 $dM_B/dt$  = the rate of change of species B (mass/time);  
 $D_A$  = decay rate of species A (1/time);  
 $R_{BA}$  = stoichiometry (moles B produced per moles A decayed);  
 $W_A$  = molecular (or atomic) weight of species A; and  
 $W_B$  = molecular (or atomic) weight of species B.



**Note:** The accuracy of the decay algorithm in GoldSim is a function of the solution precision setting (high, medium or low) defined in the **Contaminant Transport** tab of the Options dialog (accessed from the main menu by selecting **Model | Options**).

### Simulating Radioactive Species

The GoldSim RT Module provides some specialized features to assist in simulation of radioactive species. For practical reasons, you may often wish to enter and present inventories, concentrations, quantities and flux rates for radioactive species in terms of *activity*. As used here, the activity of a radioactive species represents the number of disintegrations per unit time (and should not be confused with the thermodynamic activity of a species).

To facilitate this, GoldSim allows you to specify that a species is radioactive. If the **Radioactive** checkbox is checked, GoldSim displays the *specific activity*. (The **Radioactive** checkbox is cleared and grayed out in the CT Module).

The specific activity has units of activity per unit mass and is computed as:

$$(\text{Avogadro's Number})(\text{Decay Rate}) / (\text{Atomic Weight})$$

Activity (disintegrations per unit time) is measured in units of Becquerels (Bq) or Curies (Ci), so specific activity has units of Bq or Ci per unit mass. A drop-down list allows you to specify which of these units you wish to use.

In addition to displaying the specific activity here, the Species element always produces a vector output consisting of the specific activities of each of the species. Note that, by definition, the specific activity of a non-radioactive species is zero.

**Read more:** [Species Outputs in the Browser](#) (page 63).

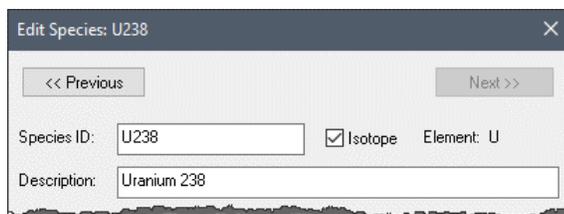


**Note:** Some radioactive species decay into multiple daughter products (e.g., 95% of the disintegrations may produce species A, and 5% may produce species B). In this case, you should use the Stoichiometry to specify this "splitting". In this example, the Stoichiometry would be 0.95 for the first daughter, and 0.05 for the second daughter.

### Simulating Isotopes of the Same Element

In some models, you may need to simulate species which are isotopes of the same element.

You specify that a species is an isotope by checking the **Isotope** check box to the right of the Species ID:



If the box is checked, the isotope's Element is displayed to the right of the Isotope check box. GoldSim defines the Element as the character(s) to the left of the first number in the species ID (e.g., the element name for Am241 would be Am). Therefore, it is recommended that isotope species be named as EE<sub>nnn</sub>, where "EE" is the element abbreviation, and "nnn" is the mass number (e.g., Am241, U238, C14).



**Note:** This is not necessary if you are using species that are included in the list from the ICRP Database provided by GoldSim within the RT Module (since GoldSim will automatically mark the appropriate species as isotopes (and identify their elements)).



**Note:** If none of the species are defined as isotopes, the Species array label set and the Elements array label set will have the same number of entries, but may be in a different order. The Elements array label set is always in alphabetical order, while the order of the Species array label set is determined by the user.

Specifying multiple species as isotopes of the same element (e.g., U235, U238) has two effects. First, isotopes of the same element are assumed to be chemically equivalent (i.e., behave identically on a molar basis with regard to partitioning, solubility, and diffusivities). These media-specific properties are defined within the Fluid and Solid media elements.

**Read more:** [Creating and Editing Environmental Media](#) (page 64).

Within a Fluid or Solid element, properties (such as solubilities and partition coefficients) can be defined by species or by element. If they are defined by species, GoldSim forces the properties of species that are isotopes of the same element to be identical. In particular, *all isotopes of the same element take on the properties of the first of the element's isotopes in the species array label set.* For example, if the species array label set included U234, U235, and U238 (in that order), all three species would use the properties (e.g., molar solubilities) assigned to U234, regardless of what was specified for the other two species.

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).

The second effect of defining multiple isotopes of the same element is related to how solubilities are computed in Cell pathways (which are the only type of transport pathway where solubility constraints can be applied). In particular, *when computing solubility constraints in Cell pathways, the solubility is "shared" by (split among) all isotopes of the same element.*

**Read more:** [Simulating Solubility Limits in Cells](#) (page 159).

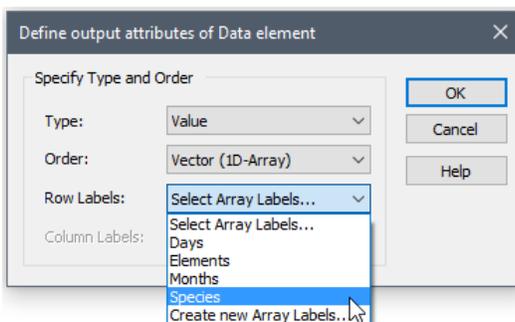
## The Species and Elements Array Label Sets

When you add, delete, or reorder species in the Species element, in addition to changing the Species element itself, you are also modifying the *Species array label set* and the *Elements array label set*.



**Note:** Array labels are discussed in "Using Vectors and Matrices" in the **GoldSim User's Guide**.

The Species and Elements array label sets are automatically created (and cannot be deleted) when you create a new file with the Contaminant Transport Module. You can use these sets when you define the output attributes for other GoldSim elements (e.g., Data, Expressions, Reservoirs):



In fact, in order to build a contaminant transport model in GoldSim, it is *required* that you do so. This is because many of the inputs to other Contaminant Transport Module elements (e.g., partition coefficients and solubilities in environmental media, mass boundary conditions in pathways, inventories for sources) require that you enter a vector by species (i.e., a vector with an item for each species) or a vector by element (i.e., a vector with an item for each chemical element).

The items in the Species array label set are the names of the species defined in the Species element. The Elements array label set is created based on the names of the chemical elements that are assigned to the species when you define their properties. If a species is not defined as an isotope (see above), the chemical element name is the species name itself. If a species is defined as an isotope, GoldSim defines the element as the character(s) to the left of the first number in the species ID (e.g., the element name for Am241 would be Am).

Unlike other array label sets in GoldSim, the Species and Array array label sets cannot be edited from the Array Labels editing dialog accessed by **Model | Array Labels**. Rather, they can only be edited via the Species element.



**Note:** You can control the order of items in the Species array label set. However, the order of items in the Elements array label set cannot be changed; the set is always in alphabetical order.



**Note:** If none of the species are defined as isotopes, the Species array label set and the Elements array label set will have the same number of entries, but may be in a different order. The Elements array label set is always in alphabetical order, while the order of the Species array label set is determined by the user.



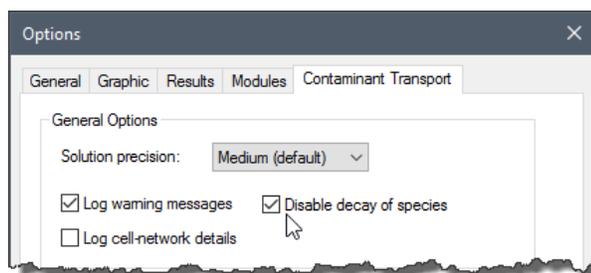
**Note:** If you are using the ICRP database of species data (available only in the RT Module), you will note that the ICRP species are shown (in the ID column) with a hyphen separating the element name from the mass number. However, within the corresponding Species array label set, the hyphen is eliminated (hence, U-238 becomes U238 in the species array label set).

**Read more:** [Reordering Species](#) (page 46); [Displaying and Using Species from the ICRP Database](#) (page 47).

## Deactivating Decay

In some situations, after defining decay rates and daughter products for your species, you may want to carry out some simulations in which the species do not decay (i.e., decay is deactivated). This is particularly useful in the early stages of your modeling effort when you are testing and debugging your model. Temporarily deactivating decay makes it much easier to interpret results and assure yourself that the model has been correctly implemented.

GoldSim provides for this on the **Contaminant Transport** tab of the Options dialog (accessed via **Model | Options**):



If you check the *Disable decay of species* box, decay will be disabled (all decay rates will be ignored and assumed to be equal to 0).

## Defining Decay Rates that Vary by Location

In general, the properties of a Species element must, by definition, be constant throughout your model (e.g., you would not want the Molecular Weight of a species to take on different values in different locations in your model!). There are situations, however, in which you may wish to vary the Decay Rate or the stoichiometry for a species spatially in your model (i.e., have it take on different values at different locations in your model). For example, you may want a species to decay only in certain pathways (e.g., a pathway representing anoxic sediments; or a pathway representing the liver in a pharmacokinetic model).

GoldSim provides a mechanism for representing such behavior.

**Read more:** [Defining Spatially Variable Decay Rates](#) (page 294).

## Importing and Exporting Species Data from/to a Spreadsheet

GoldSim allows you to export your Species data to a spreadsheet, and import the data from a spreadsheet into a GoldSim file. In most cases, you will export an existing set of Species data to a spreadsheet, and then import this same data into a new GoldSim file.



**Note:** If you choose to utilize species from the ICRP database (available only in the RT Module), and export these to a spreadsheet for use in another model, when you import these back into GoldSim, they are imported as “user-defined” species.

**Read more:** [Displaying and Using Species from the ICRP Database](#) (page 47).

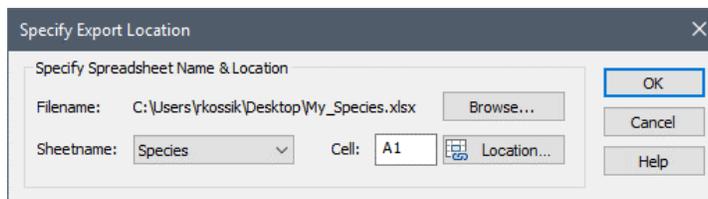
You may also choose to specify your Species data directly in a spreadsheet, and then import it into GoldSim.

The details of transferring Species data between GoldSim and a spreadsheet are discussed in the sections below.

### **Exporting Species Data to a Spreadsheet**

You can export your current Species to a spreadsheet by pressing the **Export...** button from the main Species dialog. When you do so, after a confirmation dialog, you will be asked to specify the name and location of the MS-Excel file to which you want to export the data.

You can select an existing file, or you can create a new file. After doing so, you will be presented with the following dialog:



The **Browse...** button can be used to select a different spreadsheet file. You can directly select the **Sheetname** and the starting **Cell** (the first column and row of the exported data table), or you can press the **Location...** button to directly open the spreadsheet and manually select the Cell.

Note that if you selected a new file (as opposed to an existing one), GoldSim automatically creates a sheet called "Species" in the file. The default location will then be Cell A1 in the Species sheet.

Pressing the **OK** button exports the data to the spreadsheet. An example of an exported file (Species.xlsx), illustrating the file format, can be found in the Contaminant Transport Examples folder in your GoldSim directory.

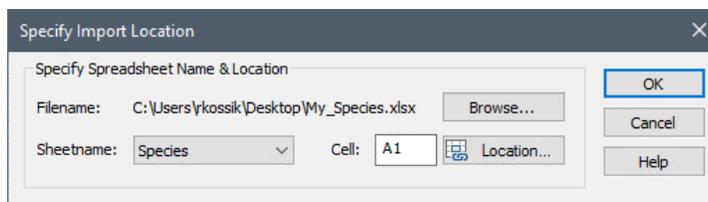
Several points should be noted regarding this file:

- The first row (specified by the row of the user-specified Cell) is used for column headers. The fourth column header can change depending on the model settings. In particular, if the decay was specified using half-lives, the column header is "Half-life". Otherwise, it is "Decay Rate".
- Checkboxes defining species properties (Radioactive, Isotope) are exported as the strings "Y" (for checked) or "N" (for unchecked).
- The spreadsheet has four columns for daughter products. Daughters set to "none" in GoldSim are exported as blank cells to the spreadsheet.
- All other data is exported as General format strings. This allows expressions and units (for the half-life/decay rate field) to be exported.

### **Importing Species Data from a Spreadsheet**

You can import Species data from a spreadsheet into GoldSim by pressing the **Import...** button from the main Species dialog. When you do so, after a confirmation dialog, you will be asked to specify the name and location of the MS-Excel file from which you want to import the data.

After selecting a file, you will be presented with the following dialog:



The **Browse...** button can be used to select a different spreadsheet file. You can directly select the **Sheetname** and the starting **Cell** (the cell containing the first column header - SpeciesID), or you can press the **Location...** button to directly open the spreadsheet and manually select the Cell.

Pressing the **OK** button imports the data from the spreadsheet into GoldSim. If the spreadsheet file was created by GoldSim (via a previous export), you do not need to worry about the format of the file, as the format for exported and imported files is identical.



**Note:** If you choose to utilize species from the ICRP database (available only in the RT Module), and export these to a spreadsheet for use in another model, when you import these back into GoldSim, they are imported as “user-defined” species.

**Read more:** [Displaying and Using Species from the ICRP Database](#) (page 47).

In some cases, however, you may wish to create the spreadsheet file directly, entering all Species data via the spreadsheet. In this case, in order to ensure that the all required columns and headers are included, it is recommended that you start with the example file (Species.xls), that can be found in the Contaminant Transport Examples folder in your GoldSim directory, and simply edit that file directly with your own data.

The following points should be noted regarding the format of the spreadsheet data that you wish to import:

- With one exception, GoldSim ignores the first row (the column headers). The exception is the cell three cells to the right of the specified starting cell location (e.g., Cell D1 if the starting location is A1). This cell *must* be a string that is either Decay Rate or Half-Life. This tells GoldSim the type of data that is being imported to define decay.
- After determining the type of decay data to be imported, GoldSim checks to be sure that the header of the fourth column of the spreadsheet data is consistent with the current setting in the main species dialog ("Decay rates" or "Half-lives"). If the spreadsheet is inconsistent with the GoldSim file, GoldSim will issue a warning message.
- The data type in the cells must be a string (General). Cells formatted as currency or date cannot be imported.
- The first column contains the Species IDs. These must be valid GoldSim species names.
- You cannot specify the same ID more than once in the spreadsheet. If you do, GoldSim will display a warning message and the second occurrence will be ignored.

- The CT Module does not support daughter products (this is only supported by the RT Module). If you are using the CT Module and try to read in species for which daughters have been specified, GoldSim will display a warning message and the daughter inputs will be ignored.

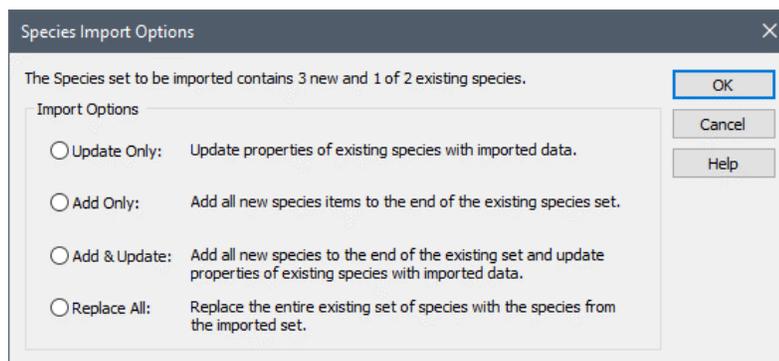
**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4).

- If you specify a daughter product that does not exist in the species list, the daughter will be ignored.

### **Replacing and Updating Existing Species During a Spreadsheet Import**

When you import Species data from a spreadsheet into GoldSim, GoldSim must decide what to do with existing Species data that may exist in the GoldSim model.

Hence, when GoldSim reads the spreadsheet, it first compares the species list currently in GoldSim to the species list being imported. It then reports how many of the species to be imported from the spreadsheet already exist in the GoldSim model and how many are new (i.e., they don't currently exist in the GoldSim model). Based on what it finds, GoldSim offers you several choices for how you want to treat the new data:



Note that depending on the data being imported and the species already in the model, not all of these options will be applicable. If they are not applicable, they will be grayed out. There are four possible combinations that can occur:

- The number and IDs of existing species exactly matches the number and IDs of species in the spreadsheet file. In this case, **Update Only** is the only available option. When you press OK, the new properties for the species in the spreadsheet will overwrite the existing properties. In this case, the order of the species in the spreadsheet is not important and the order of species in GoldSim remains unchanged.
- None of the existing species are present in the spreadsheet file. In this case, two options are presented: **Add Only** and **Replace All**. If you select **Add Only**, the new species will be added to the end of the species list (and existing species will be unchanged). If you select **Replace All**, all of the existing species will be deleted and replaced by the new species (in the order they exist in the spreadsheet file).
- Some of the existing species are present in the spreadsheet file, but there are no new IDs in the spreadsheet file that do not already exist in the existing species list. In this case, two options are presented: **Update Only** and **Replace All**. If you select **Update Only**, the new properties for the species present in the spreadsheet will overwrite the existing properties. Species not in the spreadsheet are unaffected. If you select **Replace All**, all species that are not in the spreadsheet will

be removed from GoldSim, and the remaining species will be updated with new data from the spreadsheet. During the update, the order of species in the GoldSim model (that are being updated by the spreadsheet) will not change.

- Some of the existing species are present in the spreadsheet file, but there are also species in the spreadsheet file that do not already exist in GoldSim. In this case, all four options are available. If you select **Update Only**, for species present in both the spreadsheet and the existing list, the new properties for the species present in the spreadsheet will overwrite the existing properties. Species not in the spreadsheet are unaffected. If you select **Add Only**, new species in the spreadsheet that are not already in the GoldSim file will be added to the end of the species list. All other existing species will be unchanged. If you select **Add & Update**, for species present in both the spreadsheet and the existing list, the new properties for the species present in the spreadsheet will overwrite the existing properties. In addition, new species in the spreadsheet that are not already in the GoldSim file will be added to the end of the species list. If you select **Replace All**, all species that are not in the spreadsheet will be removed from GoldSim, and the remaining species will be updated with new data from the spreadsheet. During the update, the order of species in the GoldSim model that are also present in the spreadsheet will not change.

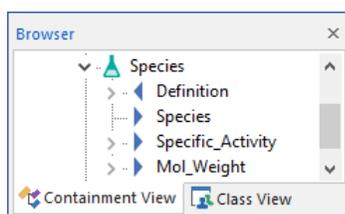


**Warning:** It is important to keep in mind that when you import new species, you are also modifying the *Species array label set* and the Elements array label set. As such, any arrays that you have created that use these sets will be impacted. For example, if you add new species, new rows would be added to a vector based on the Species array label set, and the values would default to zero (or false, if a condition).

**Read more:** [The Species and Elements Array Label Sets](#) (page 57).

## Understanding the Browser View of the Species Element

The manner in which the Species element is displayed in the browser is shown below:



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

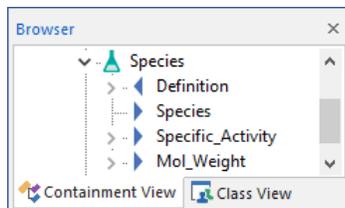


**Note:** You can review the manner in which GoldSim represents inputs and outputs to an element in the browser views (and input and output interfaces) by reading Chapter 3 of the **GoldSim User's Guide**.

### Species Outputs in the Browser

The inputs and outputs in the browser view of the Species element are discussed in detail in the topics below.

The Species element has three outputs: a special output called Species, a vector of specific activities (Specific\_Activity), and a vector of molecular weights (Mol\_Weight):



The Species output is unique, in that unlike nearly all other outputs in GoldSim, it cannot be manually linked to any input in a GoldSim model. Rather, *it is automatically linked to all pathway elements and Source elements when they are created.* That is, since all pathways and sources require as fundamental inputs the list of species being simulated and their properties, they automatically have an input (called Species) that must be linked to a Species element (this input only appears in the browser views for pathways and Sources, and does not appear in their property dialogs). When the pathway or Source is created, it automatically looks for the nearest Species element and links to it. (To represent spatial variability, some models may have multiple "clones" of the Species element. The pathway and Sources will link to the nearest Species clone in the containment hierarchy.

**Read more:** [Representing Spatial Variability](#) (page 294).

The second output produced by the Species element is a vector of specific activities called Specific\_Activity. This is a vector by species (i.e., based on the species array label set). The vector contains the specific activity of each species. The specific activity of non-radioactive species is, by definition, zero. Therefore, the Specific\_Activity output is only of use if you are simulating radioactive species. This output is useful, for example, for rapidly converting a vector of species masses to a vector of species activities.

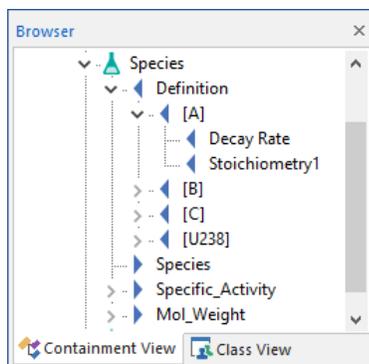
The display units for this output are specified in the Species Definition dialog. Note that if you change the specific activity display units for one species, it is changed for all species.

The third output produced by the Species element is a vector of molecular weights called Mol\_Weight. This is a vector by species (i.e., based on the species array label set). The vector contains the molecular weight of each species. This output is useful, for example, for rapidly converting a vector of mass concentrations to a vector of molar concentrations. The display units for this output are always g/mol.

In order to save the Specific\_Activity or the Mol\_Weight output as a result, you must select a save option from the context menu for this output in the browser view (accessed via a right-click on the output).

### Species Inputs in the Browser

Within the browser view, the single input to a Species element is labeled "Definition". It is a vector by species. It expands to show each of the species in the model. Of all of the properties of a particular species, only two accept links from other elements: the Half-life (or Decay Rate) and the Stoichiometries for the various daughters. Therefore, if you expand a particular species of the Definition input, only these inputs appear:



The Half-lives (or Decay Rates) and Stoichiometry are the only items in browser view for a Species element that you can link an output to (using the Link Cursor). All other Species element inputs must be specified via the species definition dialog.

## Creating and Editing Environmental Media

Environmental media (such as water, air, and soil) are the basic "building blocks" of transport pathways. For each pathway in GoldSim, you must define the environmental media which are contained in the pathway, and mass transport calculations are based, to a large extent, on the properties of these media.



There are two types of environmental media in GoldSim: *Fluids* and *Solids*.

The kinds of media represented by these two types are self-evident: Fluids are used to represent media such as water, air, oil and blood; Solids are used to represent media such as soil, rock, sediment and muscle tissue.

One of the key property sets for an environmental medium is the set of partition coefficients for the various species with respect to that medium. A partition coefficient quantifies the degree to which a species partitions between media, and is expressed as the ratio of the concentration in one medium to the concentration in another medium (at equilibrium). In GoldSim, all partition coefficients must be expressed relative to the Reference Fluid. In most cases, the Reference Fluid will be water.

### Editing the Reference Fluid

All models must contain a Reference Fluid. For convenience, the Reference Fluid is automatically provided in the Material Container, which is created in the Model Root whenever you create a new file with the Contaminant Transport Module. The default name for the Reference Fluid is "Water". If desired, you can move or rename this element, but you cannot delete it.

You cannot insert or create copies of the Reference Fluid (i.e., each model must have a single unique Reference Fluid), but in order to represent spatial variability of fluid properties, you can create *clones* of the Reference Fluid.

**Read more:** [Defining Spatially Variable Media Properties](#) (page 295).

The editing dialog for the Reference Fluid is shown below:

### Reference Fluid Properties

The Reference Fluid has four properties: a **Reference Diffusivity**, a **Diffusive Reduction Formula**, a set of **Relative Diffusivities**, and a set of **Solubilities**.

The latter two must be specified for every species. Note, however, that they are actually elemental properties, as opposed to species properties. That is, if you have defined species that represent isotopes of the same chemical element, these properties must be identical for all isotopic species of the element. (If you are not simulating isotopes, you need not be concerned with this, as there is then a one-to-one correspondence between each species and each element).

**Read more:** [The Species and Elements Array Label Sets](#) (page 57).

**Reference Diffusivity:** The reference diffusivity is the diffusivity for a "standard" or "reference" species in the fluid. It must have dimensions of area/time. As will be seen below, this "reference" value can be modified (multiplied by a specified factor) for each individual species.

**Diff. Reduction Formula:** The Diffusivity Reduction Formula is a dimensionless value that has the impact of decreasing the effective diffusivity based on the the fluid's saturation level within any Cell pathways in which it is present. This allows you to more accurately simulate diffusion through partially saturated porous media. If diffusion through partially saturated media is not of interest, simply leave this at its default value (1).

When used, this formula is intended to directly reference the fluid's saturation level using a special local available property called "Saturation". It must be referenced as "~Saturation" in the equation entered into the field. Note that the ~Saturation local available property can only be referenced directly in this field; it cannot be used in a separate element that is then linked into this field.



**Note:** Locally available properties are discussed in detail in Chapter 10 of the **GoldSim User's Guide**.

When the fluid is used within a Cell pathway, GoldSim internally computes the saturation of the fluid in the pathway, and uses this value to compute the Diffusivity Reduction Formula (and hence the diffusive mass flux) into and out of the Cell.

**Read more:** [Diffusion Through Partially Saturated Porous Media](#) (page 142).



**Note:** If the Diffusivity Reduction Formula is used (i.e., you change it from its default value of 1), you should ensure that it is defined such that it becomes 0 when the saturation is 0, and 1 when the saturation is 1.

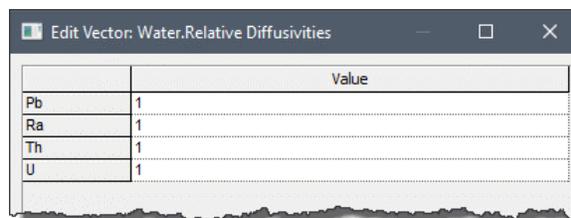
**Relative Diffusivities:** A Relative Diffusivity is unitless, and within GoldSim, is multiplied by the Reference Diffusivity to determine the actual diffusivity of each species in the fluid. This input requires that you enter a vector by element (a vector with an item for each chemical element) or a vector by species (a vector with an item for each species).

By default, the vector is defined *locally* as a vector *by (chemical) element*, which means that you can edit it directly from this dialog (by pressing the **Edit...** button to the right of the input field).



**Note:** The Elements array label set is always in alphabetical order.

This brings up the following dialog for editing the vector:



You can enter constants, expressions, or links into the fields for each element. Note that the default value for each element is 1 (i.e., the diffusivity for the element is identical to the Reference Diffusivity).

If you wish to enter a link to define the entire vector, rather than defining the vector locally, you must first press the **Clr** button. This will clear the local vector, and make the edit field available to you for entering a link. When entering a link, you can link to either to a vector by element (a vector with an item for each chemical species) or a vector by species (a vector with an item for each species). The vector must be dimensionless.



**Note:** If you are simulating isotopes of the same element, regardless of how the data is entered (by species or elements), GoldSim will automatically ensure that isotopic species use the same values for the Relative Diffusivity (if data is entered as species, the value for the first species in the list will be used for other isotopes).

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).



**Note:** If you link to a vector by species, and then subsequently decide to specify the vector locally (by pressing the **Edit...** button), the dialog for entering the data locally will be presented in terms of species. To change this back to a local vector by elements, you must first link to a dimensionless vector of elements, and then press the **Edit...** button again.

**Solubilities:** The solubility represents the maximum concentration that the chemical element can have in the Reference Fluid within a Cell pathway (with any additional mass being precipitated out of solution). This input requires that you enter a vector by element (a vector with an item for each chemical element) or a vector by species (a vector with an item for each species).

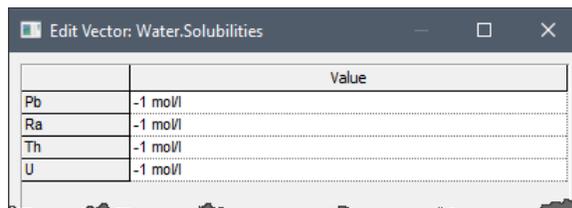
The solubility can either be specified in terms of moles/volume or mass/volume.

By default, the vector is defined *locally* as a vector *by (chemical) element*, which means that you can edit it directly from this dialog (by pressing the **Edit...** button to the right of the input field).



**Note:** The Elements array label set is always in alphabetical order.

This brings up the following dialog for editing the vector:



A negative solubility indicates that you do not wish to apply any solubility constraints for this element (i.e., the element can never become limited by solubility).

You can enter constants, expressions, or links into the fields for each element. Note that the default value for each element is -1 mol/l. GoldSim interprets a negative solubility as indicating that the chemical element is infinitely soluble (i.e., no solubility constraint will be applied).

If you wish to enter a link to define the entire vector, rather than defining the vector locally, you must first press the **Clr** button. This will clear the local vector, and make the edit field available to you for entering a link. When entering a link, you can link to either to a vector by element (a vector with an item for each chemical species) or a vector by species (a vector with an item for each species).

By default, the vector must have dimensions of moles/volume. However, by changing the **Display Units** immediately to the right of the Solubilities field, you can also choose to specify the solubilities in terms of mass/volume.



**Note:** If you link to a vector by species, and then subsequently decide to specify the vector locally (by pressing the **Edit...** button), the dialog for entering the data locally will be presented in terms of species. To change this back to a local vector by elements, you must first link to a dimensionless vector of elements, and then press the **Edit...** button again.



**Note:** If you are simulating isotopes of the same element, regardless of how the data is entered, GoldSim will automatically ensure that isotopic species use the same values for the (molar) Solubility. If data is entered as species, the molar solubility for the first species in the list will be applied to all isotopes. If the data is entered as elements, and solubilities are entered on a mass basis, a molar solubility is computed based on the Atomic Weight of the first species in the list.

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).



**Note:** Solubilities are only applied within Cell pathways (and are not applicable to any other type of pathway).

**Read more:** [Simulating Solubility Limits in Cells](#) (page 159).



**Note:** You can paste data from a spreadsheet, a Word table or a comma-delimited text file into any of the vector editing dialogs for a Reference Fluid by copying the data to the clipboard, single-clicking in the cell representing the top of the target range, and pressing **Ctrl+V**.

### **Saving Results for the Reference Fluid**

The three properties that you enter for the Reference Fluid are "passed through" the element and become outputs which you can then link to other elements.

**Read more:** [Understanding the Browser View of Media Elements](#) (page 81).

You can save these results by clicking **Final Values** and/or **Time Histories**. Checking one of these causes all three outputs to be saved as results. If you wish to save only one or two of these as results, you can use the context menu of the output (accessed via a right-click) in the browser to turn on or off one or more of the three outputs. In this case, the checkbox in the dialog would become gray (indicating that *some* of the results will be saved).

The display units for these three outputs are specified immediately to the right of the inputs (the Relative Diffusivities are dimensionless, and hence have no display units).

### **Adding and Editing Fluids and Solids**

Although you cannot add additional Reference Fluids to your model (except as clones), you can add as many Fluids and Solids as desired. To add a new Fluid or Solid:

1. Select **Model | Insert Element| Contaminant Transport | Fluid** (or) **Solid** from the main menu OR Select **Insert Element| Contaminant Transport | Fluid** (or) **Solid** from the context menu of a Container or the graphics pane.

2. Enter the Element ID and description.
3. Define the properties of the medium.

To edit an existing fluid or solid:

1. Double-click on the element in the graphics pane or the browser to access the editing dialog.
2. Define the properties of the medium.

In addition to using the editing dialog, you can also edit the properties of a medium by directly creating links to the various inputs, either in the input interface of the element in the graphics pane or the browser, using the Link Cursor.

**Read more:** [Understanding the Browser View of Media Elements](#) (page 81).

## Defining Fluids

The editing dialog for a Fluid is shown below:

The screenshot shows the 'Fluid Properties: Oil' dialog box. It has a 'Definition' tab. The 'Element ID' field contains 'Oil' and has an 'Appearance...' button next to it. The 'Description' field is empty. Under 'Fluid Properties', there are several input fields: 'Reference Diffusivity' is set to '1E-9 m2/s', 'Diff. Reduction' is '1', and 'Relative' is 'Local Vector'. There are 'Edit...' and 'Clr' buttons for the 'Relative' field. Below that, there is a 'Partition Coefficient' dropdown menu set to 'Local Vector', also with 'Edit...' and 'Clr' buttons. At the bottom, there are 'Save Results' checkboxes for 'Final Values' and 'Time History'. The dialog has 'OK', 'Cancel', and 'Help' buttons at the bottom.

The dialog is identical to that of the Reference Fluid with one exception: you have a choice of either defining solubilities or partition coefficients (for the Reference Fluid you can only specify solubilities).

In most cases, you will want to define partition coefficients (rather than solubilities) for the Fluid (and this is the default). Partition coefficients determine how species partition between the Fluid and the Reference Fluid. By definition, the solubility in the Reference Fluid, along with the partition coefficients for the Fluid relative to the Reference Fluid, automatically determine the saturation concentration in the Fluid when the solubility limit for a system containing the Fluid is reached.

In some cases, you may want to create new Fluids in which you define solubilities for the Fluids. In this case, GoldSim automatically computes the partition coefficients for the Fluid with respect to the Reference Fluid. (By definition, the partition coefficient for a species is simply the ratio of the solubility in the Fluid to the solubility in the Reference Fluid).

### **Fluid Properties**

A Fluid has four properties: a **Reference Diffusivity**, a **Diffusive Reduction Formula**, a set of **Relative Diffusivities**, and a set of **Partition Coefficients** (or **Solubilities**).

The Relative Diffusivities, Partition Coefficients and Solubilities must be specified for every species. Note, however, that they are actually elemental properties, as opposed to species properties. That is, if you have defined species that represent isotopes of the same chemical element, these properties must be identical for all isotopic species of the element. (If you are not simulating isotopes, you need not be concerned with this, as there is then a one-to-one correspondence between each species and each element).

**Read more:** [The Species and Elements Array Label Sets](#) (page 57).

**Reference Diffusivity:** The reference diffusivity is the diffusivity for a "standard" or "reference" species in the fluid. It must have dimensions of area / time. As will be seen below, this "reference" value can be modified (multiplied by a specified factor) for each individual species.

**Diff. Reduction Formula:** The Diffusivity Reduction Formula is a dimensionless value that has the impact of decreasing the effective diffusivity based on the the fluid's saturation level within any Cell pathways in which it is present. This allows you to more accurately simulate diffusion through partially saturated porous media. If diffusion through partially saturated media is not of interest, simply leave this at its default value (1).

When used, this formula is intended to directly reference the fluid's saturation level using a special local available property called "Saturation". It must be referenced as "~Saturation" in the equation entered into the field. Note that the ~Saturation local available property can only be referenced directly in this field; it cannot be used in a separate element that is then linked into this field.



**Note:** Locally available properties are discussed in detail in Chapter 10 of the **GoldSim User's Guide**.

---

When the fluid is used within a Cell pathway, GoldSim internally computes the saturation of the fluid in the pathway, and uses this value to compute the Diffusive Reduction Formula (and hence the diffusive mass flux) into and out of the Cell.

**Read more:** [Diffusion Through Partially Saturated Porous Media](#) (page 142).



**Note:** If the Diffusive Reduction Formula is used (i.e., you change it from its default value of 1), you should ensure that it is defined such that it becomes 0 when the saturation is 0, and 1 when the saturation is 1.

---

**Relative Diffusivities:** A Relative Diffusivity is unitless, and within GoldSim, is multiplied by the Reference Diffusivity to determine the actual diffusivity of each species in the fluid. This input requires that you enter a vector by element (a vector with an item for each chemical element) or a vector by species (a vector with an item for each species).

By default, the vector is defined *locally* as a vector *by (chemical) element*, which means that you can edit it directly from this dialog (by pressing the **Edit...** button to the right of the input field).



**Note:** The Elements array label set is always in alphabetical order.

This brings up the following dialog for editing the vector:



You can enter constants, expressions, or links into the fields for each element. Note that the default value for each element is 1 (i.e., the diffusivity for the element is identical to the Reference Diffusivity).

If you wish to enter a link to define the entire vector, rather than defining the vector locally, you must first press the **Clr** button. This will clear the local vector, and make the edit field available to you for entering a link. When entering a link, you can link to either to a vector by element (a vector with an item for each chemical species) or a vector by species (a vector with an item for each species). The vector must be dimensionless.



**Note:** If you are simulating isotopes of the same element, regardless of how the data is entered (as species or elements), GoldSim will automatically ensure that isotopic species use the same values for the Relative Diffusivity (if data is entered as species, the value for the first species in the list will be used for other isotopes).

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).



**Note:** If you link to a vector by species, and then subsequently decide to specify the vector locally (by pressing the **Edit...** button), the dialog for entering the data locally will be presented in terms of species. To change this back to a local vector by chemical elements, you must first link to a dimensionless vector of elements, and then press the **Edit...** button again.

**Partition Coefficients:** The partition coefficient is defined as the ratio, at thermodynamic equilibrium, of the concentration in the Fluid to that in the Reference Fluid. The partition coefficient for a Fluid is dimensionless. This input requires that you enter a dimensionless vector by element (a vector with an item for each chemical element) or a vector by species (a vector with an item for each species).

By default, the vector is defined *locally* as a vector *by (chemical) element*, which means that you can edit it directly from this dialog (by pressing the **Edit...** button to the right of the input field).



**Note:** The Elements array label set is always in alphabetical order.

This brings up the following dialog for editing the vector:



You can enter constants, expressions, or links into the fields for each element. Note that the default value for partition coefficients is zero (i.e., species do not partition into the fluid).

If you wish to enter a link to define the entire vector, rather than defining the vector locally, you must first press the **Clr** button. This will clear the local vector, and make the edit field available to you for entering a link. When entering a link, you can link to either to a vector by element (a vector with an item for each chemical species) or a vector by species (a vector with an item for each species).



**Note:** If you link to a vector by species, and then subsequently decide to specify the vector locally (by pressing the **Edit...** button), the dialog for entering the data locally will be presented in terms of species. To change this back to a local vector by elements, you must first link to a dimensionless vector of elements, and then press the **Edit...** button again.



**Note:** If you are simulating isotopes of the same element, regardless of how the data is entered, GoldSim will automatically ensure that isotopic species use the same values for the (molar) Solubility. If data is entered as species, the molar solubility for the first species in the list will be applied to all isotopes. If the data is entered as elements, and solubilities are entered on a mass basis, a molar solubility is computed based on the Atomic Weight of the first species in the list.



**Note:** For a gas, the partition coefficient with respect to water is sometimes referred to as the *Henry's Law constant*.

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).

**Solubilities:** Rather than entering the partition coefficients for a Fluid, you can alternatively enter the solubility.

The solubility represents the maximum concentration that the chemical element can have in the Reference Fluid within a Cell pathway (with any additional mass being precipitated out of solution). This input requires that you enter a vector by element (a vector with an item for each chemical element) or a vector by species (a vector with an item for each species).

The solubility can either be specified in terms of moles/volume or mass/volume.

In this case, GoldSim automatically computes the partition coefficients for the Fluid with respect to the Reference Fluid. (By definition, the partition coefficient for a species is simply the ratio of the solubility in the Fluid to the solubility in the Reference Fluid).

By default, the vector is defined *locally* as a vector *by (chemical) element*, which means that you can edit it directly from this dialog (by pressing the **Edit...** button to the right of the input field).



**Note:** The Elements array label set is always in alphabetical order.

This brings up the following dialog for editing the vector:



*A negative solubility indicates that you do not wish to apply any solubility constraints for this element (i.e., the element can never become limited by solubility).*

You can enter constants, expressions, or links into the fields for each element. Note that the default value for each element is -1 mol/l. GoldSim interprets a negative solubility as indicating that the chemical element is infinitely soluble (i.e., no solubility constraint will be applied).

If you wish to enter a link to define the entire vector, rather than defining the vector locally, you must first press the **Clr** button. This will clear the local vector, and make the edit field available to you for entering a link. When entering a link, you can link to either to a vector by element (a vector with an item for each chemical species) or a vector by species (a vector with an item for each species).

By default, the vector must have dimensions of moles/volume. However, by changing the Display Units immediately to the right of the Solubilities field, you can also choose to specify the Solubilities in terms of mass/volume.



**Note:** If you link to a vector by species, and then subsequently decide to specify the vector locally (by pressing the **Edit...** button), the dialog for entering the data locally will be presented in terms of species. To change this back to a local vector by elements, you must first link to a dimensionless vector of elements, and then press the **Edit...** button again.



**Note:** If you are simulating isotopes of the same element, regardless of how the data is entered, GoldSim will automatically ensure that isotopic species use the same values for the (molar) Solubility (if data is entered as species, the molar solubility for the first species in the list will be applied to all isotopes).

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).



**Warning:** If you choose to specify solubilities (rather than partition coefficients) for a Fluid, and the Reference Fluid has unlimited (negative) solubilities for some of the elements, you must also specify unlimited (negative) solubilities for the same elements (and only those elements) in the Fluid. If there is an inconsistency in specifying the solubilities (i.e., unlimited solubilities in one fluid but defined solubilities in another), GoldSim will provide a fatal error message when you try to run the model.



**Note:** Solubilities are only applied within Cell pathways (and are not applicable to any other type of pathway).

---

**Read more:** [Simulating Solubility Limits in Cells](#) (page 159).

---



**Note:** You can paste data from a spreadsheet, a Word table or a comma-delimited text file into any of the vector editing dialogs for a Fluid by copying the data to the clipboard, single-clicking in the cell representing the top of the target range, and pressing **Ctrl+V**.

---

### **Saving Results for Fluids**

The three properties that you enter for a Fluid are "passed through" the element and become outputs which you can then link to other elements,

**Read more:** [Understanding the Browser View of Media Elements](#) (page 81).

You can save these results by clicking **F**inal **V**alues and/or **T**ime **H**istories. Checking one of these causes all three outputs to be saved as results. If you wish to save only one or two of these as results, you can use the context menu of the output (accessed via a right-click) in the browser to turn on or off one or more of the three outputs. In this case, the checkbox in the dialog will become gray (indicating that *some* of the results will be saved).

The display units for the Reference Diffusivity output (and Solubilities if they are specified) are defined immediately to the right of the input field (the Relative Diffusivities and Partition Coefficients are dimensionless, and hence do not have display units).

### **Defining Solids**

The editing dialog for a Solid is shown below:

Solids have two categories of properties (inputs): basic properties and advanced properties.

### Basic Solid Properties

A Solid has four basic properties: a **Dry Density**, a **Porosity**, a **Tortuosity**, and a set of **Partition Coefficients**.

**Dry (bulk) Density:** The Dry Density is defined as the mass of Solid divided by the total volume of the Solid (volume of solid plus volume of pores). It is used by Pipe and Aquifer pathways to compute retardation properties when the Solid is assigned to one of these pathway types. The Dry Density is also used if you specify fractional Available Porosities for the Solid.

**Read more:** [Using Aquifer Pathways](#) (page 174); [Using Pipe Pathways](#) (page 194); [Advanced Solid Properties](#) (page 77).



**Note:** The Dry Density is *not* the specific gravity of the solid. It is defined as  $(V_s \rho_s)/(V_s + V_v)$ , where  $V_s$  is the volume of the solids,  $V_v$  is the volume of voids, and  $\rho_s$  is the specific gravity of the solid.

**Porosity:** The Porosity is the ratio of pore volume to the total volume of the Solid. That is, it is defined as  $V_v/(V_s + V_v)$ , where  $V_s$  is the volume of the solids, and  $V_v$  is the volume of voids. This input is used when you define a diffusive flux link in which the Solid is present in one of the linked pathways and is specified as the porous medium through which the transport takes place. In this case, the Porosity and Tortuosity are multiplied by the diffusivity of the species in the fluid to determine an effective diffusivity for transport. The Porosity is also used to compute the transport properties when the Solid is assigned to an Aquifer or Pipe pathway.

**Read more:** [Understanding Diffusive Mass Flux Links](#) (page 95); [using Aquifer Pathways](#) (page 174); [Using Pipe Pathways](#) (page 194).

**Tortuosity:** The Tortuosity quantifies the degree to which diffusion is slowed down due to the tortuous path that a diffusing species must travel as

it moves through the pore space in the Solid. The tortuosity should be specified as a value which is less than or equal to one. This input is used when you define a diffusive flux link in which the Solid is present in one of the linked pathways and is specified as the porous medium through which the transport takes place. In this case, the Porosity and Tortuosity are multiplied by the diffusivity of the species in the fluid to determine an effective diffusivity for transport. Porosity is also used in matrix diffusion calculations for Pipe pathways.



**Note:** The Tortuosity is defined in different ways in different fields. Within GoldSim, it is defined such that the smaller the Tortuosity, the more tortuous the path. In some fields, the Tortuosity is defined as the inverse of how it is defined in GoldSim, such that more tortuous paths have a *higher* Tortuosity.

---

Note that the tortuosity as used by GoldSim is based on a porous medium that is fully saturated with a single fluid, typically water or air. For partially saturated media, the effective diffusivity is further reduced (by a **Diffusive Reduction Formula**, which is a property of the fluid through which the species is diffusing).

**Read more:** [Understanding Diffusive Mass Flux Links](#) (page 95); [Understanding Matrix Diffusion Zones](#) (page 206); [Reference Fluid Properties](#) (page 65).

**Partition Coefficients:** The partition coefficient is defined as the ratio, at thermodynamic equilibrium, of the concentration in the solid to that in the Reference Fluid. The partition coefficient for a solid has dimensions of volume/mass.

This input requires that you enter a vector by element (a vector with an item for each chemical element) or a vector by species (a vector with an item for each species). Partition Coefficients are actually an elemental property, as opposed to a species property. As such, they *should* be specified for every element (rather than species). GoldSim, however, allows you to enter them either by species or element. Note that if you have defined species that represent isotopes of the same chemical element, the Partition Coefficients must be identical for all isotopic species of the element (and GoldSim will enforce this). If you are not simulating isotopes, you need not be concerned with this, as there is then a one-to-one correspondence between each species and each element.

**Read more:** [The Species and Elements Array Label Sets](#) (page 57).

The dimensions of the input must be volume/mass.

By default, the vector is defined *locally* as a vector *by (chemical) element*, which means that you can edit it directly from this dialog (by pressing the **Edit...** button to the right of the input field).



**Note:** The Elements array label set is always in alphabetical order.

---

This brings up the following dialog for editing the vector:



You can enter constants, expressions, or links into the fields for each element. The default value is 0 m3/kg (elements do not partition onto the Solid).

If you wish to enter a link to define the entire vector, rather than defining the vector locally, you must first press the **Clear** button. This will clear the local vector, and make the edit field available to you for entering a link. When entering a link, you can link to either a vector by element (a vector with an item for each chemical element) or a vector by species (a vector with an item for each species).



**Note:** If you link to a vector by species, and then subsequently decide to specify the vector locally (by pressing the **Edit...** button), the dialog for entering the data locally will be presented in terms of species. To change this back to a local vector by elements, you must first link to a dimensionless vector of elements, and then press the **Edit...** button again.



**Note:** If you are simulating isotopes of the same element, regardless of how the data is entered, GoldSim will automatically ensure that isotopic species use the same values for the Partition Coefficient (if data is entered as species, the Partition Coefficient for the first species in the list will be applied to all isotopes).

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).



**Note:** You can paste data from a spreadsheet, a Word table or a comma-delimited text file into any of the vector editing dialogs for a Solid by copying the data to the clipboard, single-clicking in the cell representing the top of the target range, and pressing **Ctrl+V**.

### Advanced Solid Properties

Solids have three additional properties that are typically only required for advanced contaminant transport applications. Most users can ignore these inputs. These are accessed via the **Advanced Properties...** button:



**Available Porosities:** The Available Porosity represents the fraction of the pore volume within the Solid that is accessible to each species. The

Available Porosity is dimensionless. It must be greater than or equal to 0 and less than or equal to 1.

Available Porosities must be specified for every species. Note, however, that this is actually an elemental property, as opposed to a species property. That is, if you have defined species that represent isotopes of the same chemical element, the Available Porosities must be identical for all isotopic species of the element. (If you are not simulating isotopes, you need not be concerned with this, as there is then a one-to-one correspondence between each species and each element).

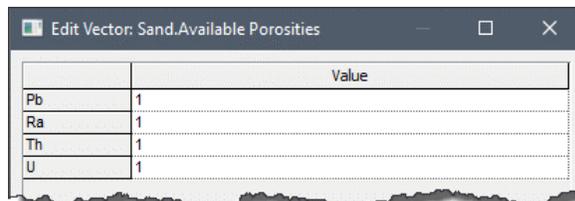
**Read more:** [The Species and Elements Array Label Sets](#) (page 57).

This input requires that you enter a dimensionless vector by element (a vector with an item for each chemical element) or a vector by species (a vector with an item for each species). By default, the vector is defined *locally* as a vector *by (chemical) element*, which means that you can edit it directly from this dialog (by pressing the **Edit...** button to the right of the input field).



**Note:** The Elements array label set is always in alphabetical order.

This brings up the following dialog for editing the vector:



You can enter constants, expressions, or links into the fields for each species. The default value is 1 (no unavailable porosity).

If you wish to enter a link to define the entire vector, rather than defining the vector locally, you must first press the **Clr** button. This will clear the local vector, and make the edit field available to you for entering a link. When entering a link, you can link to either a vector by element (a vector with an item for each chemical element) or a vector by species (a vector with an item for each species).



**Note:** If you link to a vector by species, and then subsequently decide to specify the vector locally (by pressing the **Edit...** button), the dialog for entering the data locally will be presented in terms of species. To change this back to a local vector by elements, you must first link to a dimensionless vector of elements, and then press the **Edit...** button again.

An available porosity less than 1 indicates that some of the pore volume is inaccessible for that species. Implementing an available porosity which is less than 1 may be appropriate when simulating Cell Pathways involving media such as clay, where processes such as anion exclusion may be active. For most applications, however, the available porosities should be left at the default value of 1 (i.e., no inaccessible porosity). This input requires that you enter a vector by species (a vector with an item for each species).

The Available Porosity of an element defines the fraction of the pore volume within the solid medium which is accessible to that element. The impact of specifying a fractional available porosity for a solid on mass transfer rates is complex:

- For diffusive mass flux links (and matrix diffusion zones) in which the Solid is specified as the porous medium, the effective diffusivity for the element of interest is multiplied (reduced) by the Accessible Porosity.
- The volume of water available to the species is reduced. This in turn affects the concentration (and hence the concentration gradient for diffusive mass flux links). Moreover, decreasing the volume of water available increases the retardation due to sorption (since all of the mass of the porous medium is still assumed to be available, but only a fraction of the water is).

The details regarding the manner in which inaccessible porosity affects mass transport are discussed in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).



**Note:** If you are simulating isotopes of the same element, regardless of how the data is entered, GoldSim will automatically ensure that isotopic species use the same values for the Available Porosity (if data is entered as species, the Available Porosity for the first species in the list will be applied to all isotopes).

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).

**Relative Particulate Diffusivity:** You can specify that a Solid is present in a Cell pathway as a suspended particulate. In such a case, the particulate can diffuse through a diffusive mass flux link, carrying sorbed species. This input represents the relative diffusivity of the *particulate form* of the Solid. The same value is applied to all Fluids in which the Solid is suspended. Similar to the relative diffusivity for a species, the relative diffusivity for a particulate Solid is unitless, and is multiplied by the Reference Diffusivity of the corresponding Fluid to determine the actual diffusivity of the particulate form of the Solid in the Fluid.

**Read more:** [Defining Suspended Solids in a Cell](#) (page 124); [Diffusion of Particulates to/from Cells](#) (page 141); [Advection and Diffusion of Particulates to/from Aquifers](#) (page 189).

**Advective Velocity Multiplier:** You can specify that a Solid is present in a Pipe, Cell or Network pathway as a suspended particulate. In such a case, the particulate can advect (and, in the case of Pipes and Network pathways, disperse) through an advective mass flux link from the pathway, carrying sorbed species. This input allows you to specify a factor that controls the velocity of the advected particulate Solid relative to the advecting Fluid. The default value is 1 (it moves at the same velocity as the Fluid). But you can choose to have the suspended Solid move faster or slower than the Fluid.

**Read more:** [Simulating Suspended Solids in a Pipe](#) (page 212); [Advection of Particulates to/from Cells](#) (page 138); [Simulating Suspended Solids in an Aquifer](#) (page 185).

### Saving Results for Solids

The properties that you enter for a Solid are "passed through" the element and become outputs which you can then link to other elements.

**Read more:** [Understanding the Browser View of Media Elements](#) (page 81).

You can save these results by clicking **Final Values** and/or **Time Histories**. Checking one of these causes all three outputs to be saved as results. If you wish to save only one or two of these as results, you can use the context menu of the output (accessed via a right-click) in the browser to turn on or off one or more of the three outputs. In this case, the checkbox in the dialog will become gray (indicating that *some* of the results will be saved).

The display units for the outputs are specified immediately to the right of the input field (the Porosity, Tortuosity, Available Porosities and Relative Particulate Diffusivity are dimensionless, and hence do not have display units).

### Entering Media Properties for Isotopes of the Same Element

There are four media properties that must be specified for each species in the model:

- Solubilities in the Reference Fluid (and optionally, for other fluids);
- Partition Coefficients for other Fluids and Solids;
- Relative Diffusivities for Fluids; and
- Available Porosities for Solids.

If you define multiple isotopes of the same element, GoldSim treats these four properties in a special way: isotopes of the same element are assumed to have equivalent properties. If the properties are defined by element (the default), this is straightforward (as isotopes of the same element are represented by a single entry). However, you can optionally define these properties individually for each species. In this case, it is possible that they could be entered inconsistently (i.e., isotopes of the same element could be assigned different values).

In this case, within a Fluid or Solid element, GoldSim forces the properties for isotopes of the same element to be equivalent. In particular, *all isotopes of the same element take on the properties of the first of the element's isotopes in the species array label set*. For example, if the species array label set included U234, U235, and U238 (in that order), all three species would use the properties assigned to U234, *regardless of what was specified for the other two species*.



**Note:** When specifying solubilities, GoldSim requires that the *molar* solubilities of all isotopes of an element are identical. By default, solubilities are specified as molar solubilities. Note, however, that solubilities can optionally be specified on a mass basis (e.g., mg/l). In this case, the mass-based solubilities of isotopes of an element should be specified as being proportional to the atomic weights of the isotopes. For example, if you have two isotopes of an element with atomic weights 238 and 234, and the solubility of the first isotope is specified as 1 mg/l, then the solubility of the second isotope should be specified as (234/238) mg/l. If it is not, GoldSim will automatically correct the problem (using the molar solubility defined by the first isotope), and will write a warning message to the Run Log.

---

An important effect of defining multiple isotopes of the same element is related to how solubilities are computed in Cell pathways (which are the only type of transport pathway where solubility constraints can be applied). In particular, *when computing solubility constraints in Cell pathways, the solubility is "shared" by (split among) multiple isotopes of the same element*.

## Understanding the Browser View of Media Elements

**Read more:** [Simulating Solubility Limits in Cells](#) (page 159).

Although you may choose to edit the media elements only through the editing dialogs, when an input to a medium is a link from other elements in the model, you may prefer to create the link via the browser view and/or the input interface to the medium. In addition, experienced users may find it more convenient to create links from media elements using the browser or the output interface. This section discusses the browser view for each of the medium elements (recall that the input and output interfaces to an element are simply partial copies of the browser view).



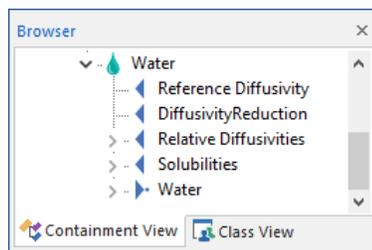
**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).



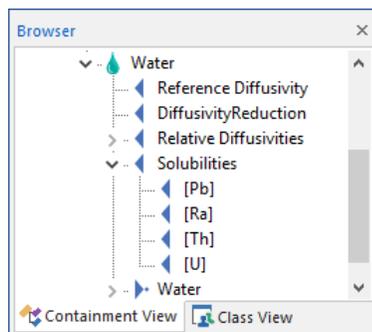
**Note:** You can review the manner in which GoldSim represents inputs and outputs to an element in the browser views (and input and output interfaces) by reading Chapter 3 of the **GoldSim User's Guide**, "Building a Model in GoldSim".

## Reference Fluid Inputs and Outputs in the Browser

The browser view of the Reference Fluid is shown below:



All three inputs to the Reference Fluid can be specified as links, and hence all three appear in the browser. The Relative Diffusivities and Solubilities are vectors (by element), and hence can be expanded:



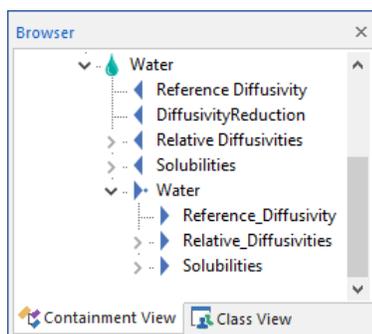
The Reference Fluid has a single output (and hence has the same ID as the medium). When a pathway is created, it is automatically linked to this output (you cannot do this manually).



**Note:** In some instances, to represent spatial variability, some models may have multiple "clones" of the Reference Fluid element. The pathways will link to the nearest Reference Fluid clone in the containment hierarchy.

**Read more:** [Defining Spatially Variable Media Properties](#) (page 295).

The Reference Fluid output expands to reveal the medium properties, as shown below:



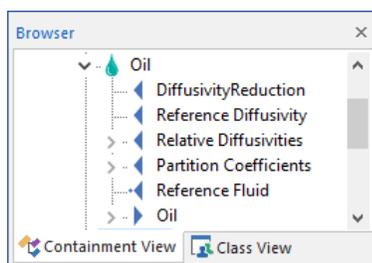
*The Relative Diffusivities and Solubilities outputs are vectors. You can create a link from the entire vector, or expand the output and create a link from an item of the vector.*

That is, the three properties that you enter for the Reference Fluid are "passed through" the element and become outputs which you can then link to other elements.

You can save these results by clicking **Final Values** and/or **Time Histories** in the editing dialog for the Reference Fluid. Checking one of these causes all three outputs to be saved as results. If you wish to save only one or two of these as results, you can use the context menu of the output (accessed via a right-click) in the browser to turn on or off one or more of the three outputs. In this case, the checkbox in the editing dialog would become gray (indicating that *some* of the results will be saved).

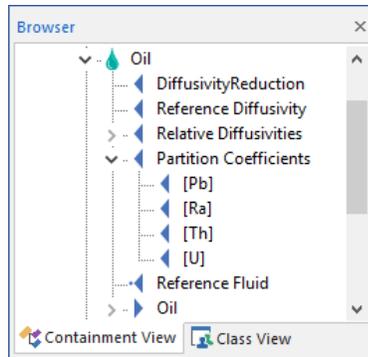
### Fluid Inputs and Outputs in the Browser

The browser view of a Fluid is shown below:

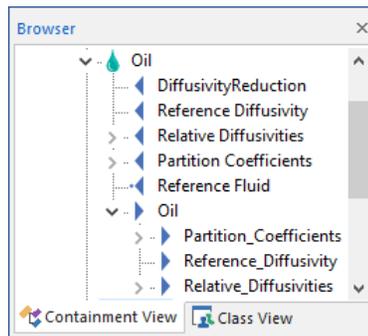


Note that the Reference Fluid appears as an input. This input is automatically linked to the Reference Fluid (or the nearest clone of the Reference Fluid) when the Fluid is created. *This link cannot be changed using the Link Cursor, and is displayed for information purposes only.*

The other three inputs to the Fluid can be specified as links. The Relative Diffusivities and Partition Coefficients (or alternatively, Solubilities) are vectors (by element), and hence can be expanded:



A Fluid has a single output (and hence has the same ID as the medium). The Fluid output expands to reveal the medium properties, as shown below:



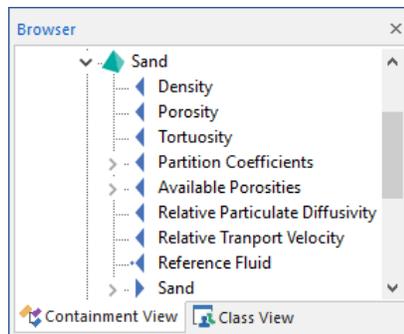
The Partition Coefficients and Relative Diffusivities outputs are vectors. You can create a link from the entire vector, or expand the output and create a link from an item of the vector.

That is, the three properties that you enter for a Fluid are "passed through" the element and become outputs which you can then link to other elements.

You can save these results by clicking **Final Values** and/or **Time Histories** in the editing dialog for the Fluid. Checking one of these causes all three outputs to be saved as results. If you wish to save only one or two of these as results, you can use the context menu of the output (accessed via a right-click) in the browser to turn on or off one or more of the three outputs. In this case, the checkbox in the editing dialog would become gray (indicating that *some* of the results will be saved).

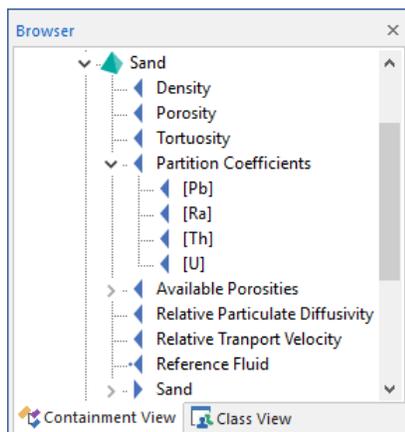
### Solid Inputs and Outputs in the Browser

The browser view of a Solid is shown below:

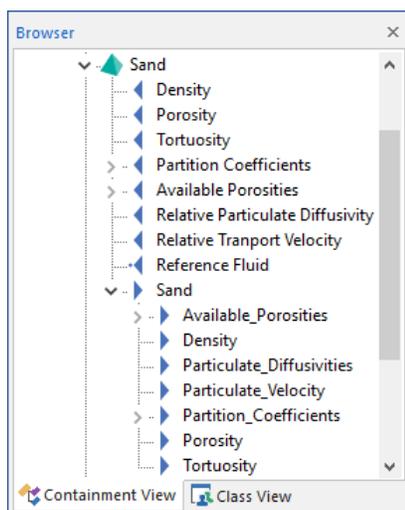


Note that the Reference Fluid appears as an input. This input is automatically linked to the Reference Fluid (or the nearest clone of the Reference Fluid) when the Solid is created. *This link cannot be changed using the Link Cursor, and is displayed for information purposes only.*

The other inputs to the Solid can be specified as links. The Available Porosities and Partition Coefficients are vectors (by element), and hence can be expanded:



A Solid has a single output (and hence has the same ID as the medium). The Solid output expands to reveal the medium properties, as shown below:



The Available Porosities and Partition Coefficients outputs are vectors. You can create a link from the entire vector, or expand the output and create a link from an item of the vector.

That is, each of the properties that you enter for a Solid are "passed through" the element and become outputs which you can then link to other elements.

You can save these results by clicking **Final Values** and/or **Time Histories** in the editing dialog for the Solid. Checking one of these causes all outputs to be saved as results. If you wish to save only one or several of these as results, you can use the context menu of the output (accessed via a right-click) in the browser to turn on or off one or more of the outputs. In this case, the checkbox in the editing dialog would become gray (indicating that *some* of the results will be saved).

## Representing Spatial Variability in Media Properties

In many cases, you will want the properties of the environmental media in your model to vary spatially. For example, the solubility for a species in Water or the partition coefficient for a species in Sand may take on different values in different locations (pathways) in your model.

GoldSim provides a mechanism for representing such behavior. In general, it involves either using different media in different locations (e.g., defining two

types of Sand) or creating "clones" of a single medium, which take on different values in different locations.

*Read more:* [Defining Spatially Variable Media Properties](#) (page 295).

## Copying Material Elements Between GoldSim Model Files

In many cases, you may wish to create different portions of your model in different model files. For example, one individual may be working on one part of your model (a particular subsystem), while another is working on a different subsystem. At some point, you would then want to combine the various subsystems into a single model file.

GoldSim allows you do so by simply opening two instances of GoldSim (each with a different file), copying the desired elements (including entire Containers) to the clipboard, and then pasting them into the other model. Copying elements between models in this way is discussed in detail in Chapter 3 of the **GoldSim User's Guide**, "Building a Model in GoldSim".

When you are copying and pasting Material elements in this manner, however, there are several limitations that GoldSim imposes that you must be aware of:

- You cannot copy the Species element between models. If you try to copy a Container containing the Species element, GoldSim will issue a warning message and prevent you from doing so.
- You can only copy Fluids and Solids between models if the two models have species lists with the same *number* of species and the same number of chemical elements (although the species and element *names* do not have to be identical). This is because Fluids and Solids use the species and elements array label sets. If the number of species or the number of elements was different between models, it would cause a conflict when the Fluid or Solid element was pasted, and GoldSim therefore prevents you from doing so.



**Note:** When Containers are pasted into the same scope from which they were copied, GoldSim always localizes them. As a result, other elements will not be able to see items in the Container unless you globalize it or expose the inputs. Localizing Containers and exposing outputs is discussed in Chapter 10 of the **GoldSim User's Guide**, "Advanced Modeling Concepts".

---



---

# Chapter 4: Transport Pathways

Look at every path closely and deliberately. Try it as many times as you think necessary. Then ask yourself, and yourself alone, one question ... Does this path have a heart? If it does, the path is good; if it doesn't, it is of no use.

Carlos Castaneda, *The Teachings of Don Juan*

## Chapter Overview

This chapter describes the central component of a contaminant transport model, the transport pathway. A contaminant transport model is constructed by defining multiple transport pathways and linking them together into an interconnected network.

Transport pathways represent physical components through which species can move (and/or be stored) such as aquifers, lakes, sediments, surface soil compartments, and the atmosphere. In order to represent the wide variety of transport pathways which you may wish to simulate, GoldSim provides four different kinds of pathway elements: 1) Cell pathways; 2) Pipe pathways; 3) External pathways; and 4) Network pathways. These pathways can be used interchangeably within a model.

### In this Chapter

This chapter discusses the following:

- Understanding Transport Pathways
- Creating Mass Flux Links
- Using Cell Pathways
- Using Aquifer Pathways
- Using Pipe Pathways
- Using External Pathways
- Using Network Pathways
- Additional Comments on the Use of Transport Pathways
- References

## Understanding Transport Pathways

### What is a Transport Pathway?

A transport pathway can be thought of as a *transfer function* (i.e., an operator), whose input is a mass flux rate and whose output is a mass flux rate:



The transport pathway operates on (i.e., delays, spreads, reduces, magnifies) incoming mass fluxes in order to produce a time history of outgoing mass fluxes from the pathway. In the absence of decay, transport pathways conserve the mass of contaminant within a system.



**Note:** Although it is convenient to think of all pathways as transfer functions, this description is not strictly mathematically accurate for Cell pathways that are part of a larger *Cell net*.

**Read more:** [Understanding Cell Nets](#) (page 165).

Physically, transport pathways represent the components of a system through which mass (e.g., contaminant species) can move and/or be stored. Typically, a pathway will represent all or part of an environmental component, such as an aquifer, stream, soil compartment, lake, or a portion of the atmosphere. You define the properties of the pathways, such as their geometry and which environmental media (e.g., water, air, soil) they contain.

In order to represent the wide variety of transport pathways which you may wish to simulate, GoldSim provides five different pathway element types, which can be used interchangeably in a model:

### Types of Pathway Elements



**Cell pathways** act as mixing cells. Within a Cell, all species mass is assumed to be instantaneously and completely mixed and equilibrated among all of the Cell's media. Solubility constraints can be imposed within Cell pathways. When multiple Cells are linked together, the behavior of the Cell network is mathematically identical to a network of finite difference nodes describing a coupled system of differential equations.



**Aquifer pathways** are used to represent features that essentially behave as fluid conduits or stream tubes. An Aquifer pathway actually performs its computations by creating a temporary set of linked Cell elements during the simulation, which are subsequently removed at the end of the simulation. They can be applied to a broad range of advectively-dominated mass transport systems involving one-dimensional advection, longitudinal dispersion, diffusion, retardation, decay and ingrowth.



**Pipe pathways** are also used to represent features that essentially behave as fluid conduits or stream tubes. Pipe pathways use a Laplace transform approach to provide analytical solutions to a broad range of advectively-dominated mass transport systems. Because they can represent processes such as matrix diffusion, they are particularly applicable to modeling transport through fractured rock masses.



**External pathways** provide a mechanism by which external program modules for mass transport (e.g., analytical, finite element or finite difference transport models) can be directly integrated into GoldSim. The modules are linked into GoldSim as DLLs (Dynamic Link Libraries) at run time.



**Network pathways** provide a computationally efficient way to simulate large, complex networks of one-dimensional "pipes" in order to describe mass transport through fractured rock systems. Network pathways require specification of a separate fracture network, which typically would be generated by a discrete fracture network generation and flow simulation code. The fracture network can be very large (100,000 pipes or more), allowing complex and realistic fracture systems to be simulated. Network pathways are only available in the RT Module.

### Comparing Pipes and Aquifers

Aquifer and Pipe pathways are both intended to represent a feature that essentially behaves as a *fluid conduit*. They provide a way to simulate processes such as vertical transport through an unsaturated (vadose) zone or horizontal transport in aquifers, rivers, channels and pipelines.

Under what circumstances should one pathway be used instead of the other? Some general rules are provided below:

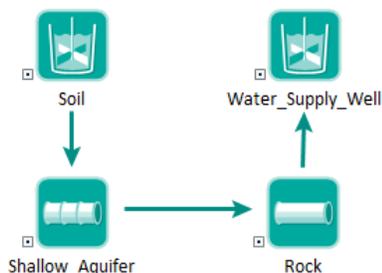
- If solubility limits are being approached within the pathway, you should use an Aquifer.
- If the pathway (or solute) properties, including flow rates, are changing significantly over the simulation, you should use an Aquifer.
- If you need to simulate processes that occur in fractured rock masses, such as matrix diffusion, you should use a Pipe.

If none of the above conditions occur, then either a Pipe or an Aquifer could be used.

**Read more:** [Using Pipe Pathways](#) (page 194); [Using Aquifer Pathways](#) (page 174); [Comparison of Aquifers and Pipes for Simulating a One-Dimensional Pathway](#) (page 251).

### Creating Pathway Networks

A model of an environmental system is created by linking pathway elements together into a pathway network, as shown below:



GoldSim moves mass through the network, keeping track of the temporally varying amount of mass in each pathway.

To create such a network, individual pathways are connected via mass flux links. A mass flux link controls the rate at which species are moving between pathways. The mass flux is a vector by species (i.e., it has one item for each species), since the flux will differ for each species being simulated, and has dimensions of mass/time.



**Note:** The Contaminant Transport Module relies heavily on GoldSim's ability to create and manipulate vectors. If you are not comfortably familiar with this capability of GoldSim, see "Using Vectors and Matrices" in the **GoldSim User's Guide**.

Two major types of mass flux links and three special purpose mass flux links can be defined in GoldSim. In an *advective mass flux link*, a quantity of a medium is specified to flow from one pathway to another, carrying dissolved, sorbed, and/or suspended species with it. In a *diffusive mass flux link*, species diffuse between pathways according to a concentration gradient. Three special purpose mass flux links allow you to model processes that cannot be represented as using advection or diffusion. In a *direct transfer mass flux link*, species are moved from one pathway to another based on a user-specified transfer rate. In a *precipitate removal mass flux link*, species present as precipitated mass are moved from one pathway to another based on a specified transfer rate. In a *treatment mass flux link*, species are treated or filtered and are moved from one pathway to another based on a specified treatment efficiency (a fraction).

Based on the properties of each pathway, the media in each pathway, the species, and the specified mass flux links, GoldSim computes the amount of mass in each pathway, the concentrations in each pathway's media, and the mass fluxes between pathways, all of which vary with time. Hence, the fundamental output of a pathway element is a series of vectors: the mass (of each species) in the pathway, the mass flux (of each species) to each of the pathways to which it is connected via mass flux links, and the concentrations (of each species) within the environmental media in the pathway.

## Creating Mass Flux Links

Because mass flux links are specified in the same way for all types of pathways, and because pathway behavior is primarily controlled by the manner in which the mass flux links between pathways are defined, it is useful to first discuss the creation of mass flux links before describing the five types of pathways in detail.

### Understanding Advective Mass Flux Links

Advective mass flux links are used to transport mass via a flowing medium. They are defined by specifying that a quantity of medium is moving (flowing) from one location to another. Species mass which is dissolved, suspended or otherwise associated with the medium is transported with the medium as it moves. Hence, an advective mass flux is computed as the concentration of the mass in the medium multiplied by the rate at which the medium is flowing:

$$\text{Advective Mass Flux} = \text{Concentration} * \text{Flow Rate}$$

Typically, the medium is a fluid, such as water. For example, suppose that you were simulating nutrient concentrations in a lake that was fed by two streams, and which discharged to a small river. The lake and streams would be represented by pathway elements. To define the inflows to the lake, you would create two advective mass flux links (one for each stream) *from* the two stream pathways *to* the lake. You would define the outflow from the lake by creating an advective mass flux link *from* the lake *to* a pathway representing the river.

Similarly, if you were simulating the transport and fate of a drug within the body (pharmacokinetic modeling), you might create advective mass flux links between pathways representing the various organs (e.g., liver, lungs) in which the fluid being advected was blood.

Although you will typically move fluids through mass flux links, in some cases it may be appropriate for the moving medium to be a solid. For example, you could model the deposition and resuspension of sediments in a lake using advective mass flux links. Any contaminants associated with (sorbed onto) the sediments would be transported with them. The movement of soil (via erosion) and the transport of contaminants associated with the soil could also be simulated using advective mass flux links involving solids.



**Note:** The Contaminant Transport Module is a mass transport model, *not* a flow model. That is, it does not directly solve for the movement of media through the environmental system being modeled. Hence, you must directly enter the media flow rates associated with an advective flux link (or provide GoldSim with the equations for computing them).

**Read more:** [Mass Balance of Transport Media in Pathway Networks](#) (page 253).

### Creating and Editing Advective Mass Flux Links

To create an advective mass flux link between two pathways in GoldSim, you must specify two things:

- The medium flowing between the pathways. This can be a fluid or a solid.
- The flow rate of the medium. This is specified in terms of volume/time for fluids and mass/time for solids.

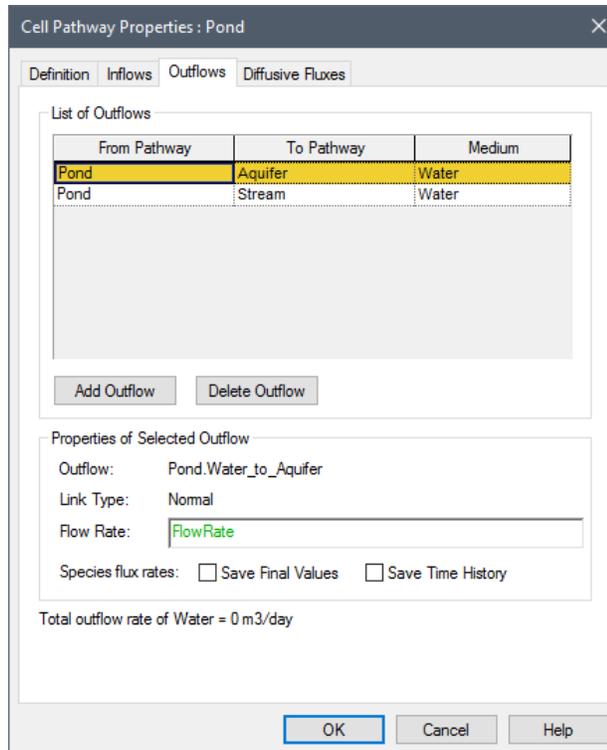
GoldSim provides two ways to create an advective flux link between two pathways:

- By using the **Outflows** tab on the pathway editing dialog; and
- By using the **Inflows** tab on the pathways editing dialog.



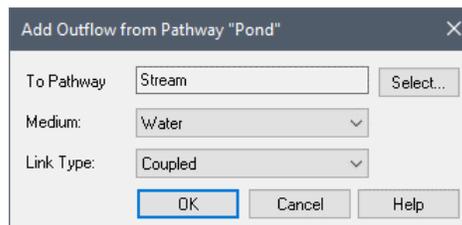
The **Outflows** tab is used to create advective flux links *from* the current pathway *to* other pathways in the model. The **Inflows** tab is used to create advective flux links *to* the current pathway *from* other pathways in the model.

The two dialogs are almost identical in appearance. The **Outflows** tab is shown below:



To create a new Outflow (a mass flux link from the current pathway to another pathway), do the following:

1. Double-click on a pathway to display the pathway editing dialog.
2. Click on the **Outflow** tab.
3. Press the **Add Outflow** button. This will bring up a browser showing all of the other pathways (or Containers with pathways) in the model.
4. Select the pathway you wish to link to and press **OK**.
5. GoldSim will then display a dialog for selecting the medium involved in the mass flux link:



*If you change your mind or have selected the wrong pathway, press the **Select...** button to change the pathway.*

The second field in this dialog is a drop list containing the Reference Fluid in the Outflow ("from") pathway, as well as any other media that the two pathways have in common.



**Note:** The Medium drop list will also include options for “Direct transfer rate”, “Precipitate transfer rate” and “Fraction of inflows”. If one of these are selected, the flux link becomes a special purpose flux link rather than an advective flux link.

**Read more:** [Understanding Direct Transfer Mass Flux Links](#) (page 103); [Understanding Precipitate Removal Mass Flux Links](#) (page 107); [Understanding Fraction of Inflows \(Treatment\) Mass Flux Links](#) (page 112).

The third field in this dialog specifies the Link Type. If you are connecting two Cells, this will default to Coupled. If the link involves any other type of pathway, it will default to Normal. In most cases, you will not need to change the field and can accept the default.

**Read more:** [Specifying the Link Type for Mass Flux Links](#) (page 118).

Select a medium and Link Type and press **OK**.

6. You will then be returned to the **Outflows** tab. Move your cursor to the Properties of Selected Outflow section and enter the **Flow Rate**. (The flow rate will be defaulted to 0 m<sup>3</sup>/s for fluids and 0 kg/s for solids.
7. If you wish to save the mass flux Final Values or Time Histories for the link, select one or both of the checkboxes.
8. Press **OK** to close the pathways dialog.

After an outflow is created, you can always change the *properties* of the outflow (i.e., the flow rate and whether or not results are to be saved) by selecting the outflow in the top of the dialog (by clicking on the appropriate row in the List of Outflows) and editing the properties in the lower section of the dialog (Properties of Selected Outflow).

The **Inflows** and **Outflows** tab only displays the pathway name, and does not indicate where the pathway exists in the model. If, however, you hold your cursor over a pathway in the list, a tooltip displays the full containment path for the pathway.



**Note:** Once an advective mass flux link is created, you cannot change the medium which is involved. The only way to change the medium is to delete the link and recreate it.

An outflow is deleted by selecting the outflow in the top of the dialog (by clicking on the appropriate row in the List of Outflows) and pressing the **Delete Outflow** button.



**Note:** To assist you in maintaining a flow balance for your model, GoldSim lists the total outflow rate of the Reference Fluid (the sum of the expected values of the outflows) at the bottom of the **Outflows** tab.

The **Inflows** tab is used to create advective flux links *to* the current pathway *from* other pathways in the model. The manner in which inflows are created,

### Inputs and Outputs Associated with Advective Mass Flux Links

edited and deleted is identical to that for outflows, and the two tabs are essentially identical in appearance.

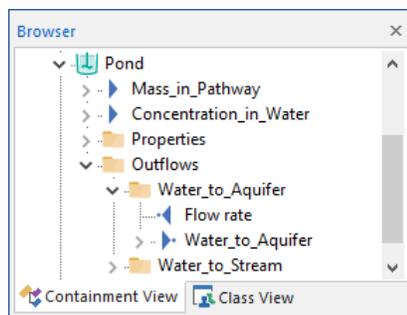
Note that when you create a mass flux link using the **Outflows** tab of one pathway, the link automatically appears in the **Inflows** tab of the linked pathway. The properties of the mass flux link can be edited from either location.

When an advective mass flux link is created, GoldSim creates several new inputs and outputs on the two linked pathways which subsequently appear in the browser view and interfaces for these pathways.

On the "from" or "outflow" pathway (the pathway from which the medium is flowing):

- GoldSim creates a new output named *Medium\_to\_Path2*, where *Medium* is the name of the flowing medium, and *Path2* is the name of the linked pathway (toward which the medium is flowing). For example, if Water was flowing from a pathway named *Aquifer* to a pathway named *Pond*, GoldSim would create a new output on the *Aquifer* pathway called *Water\_to\_Pond*. Like all GoldSim outputs, when the output appears in an expression, the name of the element is included prior to the output name (*Aquifer.Water\_to\_Pond*). This output represents the mass flux itself, and is a vector by species with dimension of mass/time.
- GoldSim creates a new input named *Flow rate*. This is the flow rate in the link. It has dimensions of volume/time for fluids and mass/time for solids.

These new items are organized under a "folder" within the browser view of the element called Outflows:

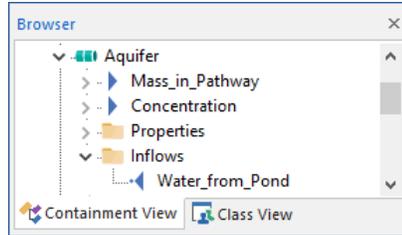


Each outflow has a separate sub-folder.

On the "to" or "inflow" pathway (the pathway to which the fluid is flowing):

- GoldSim creates a new input named *Medium\_from\_Path1*, where *Medium* is the name of the flowing medium, and *Path1* is the name of the linked pathway (from which the medium is flowing). For example, if Water was flowing from a pathway named *Aquifer* to a pathway named *Pond*, GoldSim would create a new input on the *Pond* pathway called *Water\_from\_Aquifer*. This input represents the mass flux itself, and is a vector by species with dimension of mass/time.

This new item is organized under a "folder" within the browser view of the element called Inflows:



These new items in the browser views of the pathways are useful because they can be used in conjunction with the Link Cursor to create links. For example, rather than editing the flow rate in the link using the editing dialog, you could create a link to *Flow rate* using the Link Cursor. Similarly, you could link the mass flux output itself into an Expression element, a Sum element or an Extrema element.

**Read more:** [Manipulating Pathway Outputs](#) (page 253).



**Note:** If you create multiple advective fluxes between the same two Cells, GoldSim will append the letter “c” and a number to the end of the input and output names. For example, if a second advective flux was added from Cell Aquifer to Cell Pond, the output on the Aquifer Cell would be named “Water\_to\_Pondc2” and the input on the Pond Cell would be “Water\_from\_Aquiferc2”.

### **Directionality of Advective Mass Flux Links**

In some cases, you may wish to simulate a reversal of the flow direction. For Cell Pathways, you can do this by specifying a negative **Flow Rate** for the advective flux. GoldSim treats a negative Outflow from a Cell as a positive Inflow to the Cell.

For all other Pathways, Flow Rates cannot be negative. Therefore, in order to simulate a reversal of flow direction, you must create two opposite advective flux links (with the flow rate defined using logic that ensures that it is either zero or positive).

Because advective mass flux links between Cells can be bi-directional (i.e., mass fluxes can move in either direction along the link), it is important to understand the sign convention used by GoldSim when displaying and using the advective mass flux outputs. Depending on how the link was created (in the Inflows tab or the Outflows tab), GoldSim always defines one of the two pathways as the “Outflow Pathway” and one of the pathways as the “Inflow Pathway”. Advective mass fluxes away from the Outflow Pathway are, by convention, positive, and advective mass fluxes toward the Outflow Pathway are negative.



**Warning:** Negative Flow Rates between Cell pathways are treated as positive Inflows to the originating Cell. However, negative Flow Rates to other pathways (e.g., Pipes) will generate a Fatal Error.

### **Understanding Diffusive Mass Flux Links**

Diffusive mass flux links are used to transport mass through a stagnant or slowly moving fluid via the process of molecular diffusion. Diffusive mass transport is driven by (in fact, proportional to) a concentration difference, with mass diffusing from high concentration to low concentration. The constant of proportionality is referred to as the *diffusive conductance*:

$$\text{Diffusive Mass Rate} = (\text{Diffusive Conductance}) * (\text{Concentration Difference})$$

In this equation, the Diffusive Mass Rate has dimensions of mass/time, the Diffusive Conductance has dimensions of volume/time, and the Concentration Difference has dimensions of mass/volume.

The diffusive conductance is a function of the properties of the species and fluids involved (multiple fluids can be involved), and the geometry of the diffusive process.

Assuming that the species are diffusing through a single fluid, the Diffusive Conductance term is computed as follows:

$$D = (A d t n r) / L$$

where:

- D is the Diffusive Conductance ( $L^3/T$ );
- A is the diffusive area ( $L^2$ );
- d is the diffusivity in the fluid ( $L^2/T$ );
- n is the porosity of the porous medium;
- t is the tortuosity of the porous medium;
- r is a reduction factor to account for the degree of saturation (1 if saturated);
- L is the diffusive length (L).

d and r are Fluid properties, and t and n are Solid properties.

**Read more:** [Diffusion Through Partially Saturated Porous Media](#) (page 142).



**Note:** If the diffusion is not taking place through a porous medium, t, n and r in this equation are all effectively set to 1.

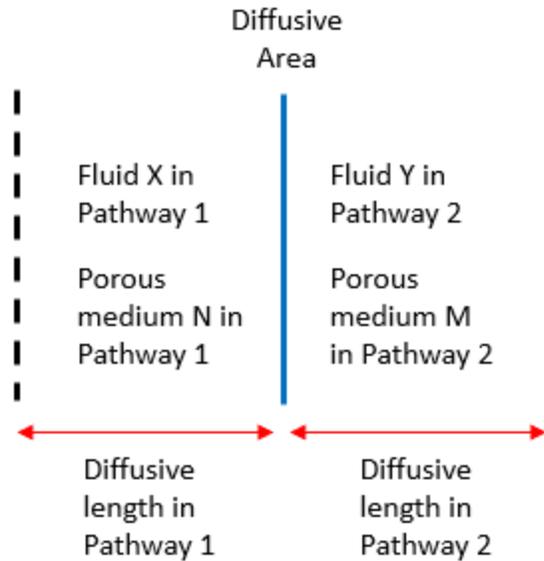
---

Diffusive mass flux links are appropriate for describing mass transport between pathways that are not dominated by advective processes. For example, if you were simulating the behavior of a landfill with a clay liner, given the low permeability of clay, the rate at which contaminants diffuse through the liner could be more significant than the rate of advective transport. In some cases, it may be appropriate to simultaneously specify advective and diffusive mass flux links (diffusion in slowly moving water).

Diffusive mass flux links may also be the most appropriate way to simulate mass transfer across fluid interfaces (e.g., the air-water interface in a lake or stream). Transport across such an interface is often mathematically represented as diffusion through two thin boundary layers (one on each side of the interface).

**Read more:** [Inter-Media Diffusion](#) (page 144).

As illustrated schematically below, a diffusive mass flux link between two pathways has two "sides" (one for each of the linked pathways). Mass diffuses from one pathway, through the "diffusive layer" on one side of the link, through the "diffusive layer" on the other side of the link, and into the other pathway.



To create a diffusive mass flux link between two pathways in GoldSim, you must do the following:

- For each side of the link, a *fluid* must be specified. Each side of the link can contain a different fluid. This determines the diffusion coefficient that is used. The diffusion coefficient can actually be species-specific.
- For each side of the link, a *diffusive length* must be specified. This length represents the thickness of the "diffusive layer". It typically represents the distance from the center of the Cell to the "edge" or interface of the Cell.
- For each side of the link, you can optionally specify a *porous medium* contained within the "diffusive layer". If you do, the diffusive flux is multiplied by the product of the porosity and the tortuosity associated with the porous medium. The porosity can actually be species-specific, while the tortuosity is assumed constant for all species.  
**Read more:** [Defining Solids](#) (page 74).
- A single *diffusive area* for the link must be specified.

These inputs, along with the properties of the fluids and porous media involved, determine the value of the diffusive conductance. (For details on the manner in which diffusive mass flux links are represented mathematically, see Appendix B).

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

Typically the fluids on the two sides of the link will be identical (e.g., water), but they do not have to be (e.g., you could simulate diffusive transport across the air-water interface). The diffusive lengths on the two sides of the link do not have to be the same. In fact, in some cases, only one "diffusive layer" may be present (the diffusive length may be assumed to be 0 on one side of the link).

Mass transport in a diffusive mass flux link between two Cells can be bi-directional. That is, species can be transported in either direction along the link. The species always diffuse from high concentration to low concentration. In some cases, therefore, at a given time, different species may be diffusing in opposite directions within the same diffusive mass flux link.

The diffusive lengths and the diffusive area control the geometry of the link. Through appropriate specification of these inputs, nearly any diffusion geometry can be represented (e.g., linear, radial, spherical).

There is one important limitation on how diffusive mass flux links can be created: *All diffusive mass flux links must originate in a Cell pathway.* This is because, by definition, GoldSim does not allow mass to diffuse *out of* non-Cell (Aquifer, Pipe, External and Network) pathways. Within GoldSim, *the concentration and diffusive length on the non-Cell side of a diffusive mass flux link are assumed to be zero.* Hence, diffusive mass flux links involving non-Cell pathways are uni-directional. A diffusive mass flux link can only be bi-directional if it is between two Cell pathways.



**Note:** Although you cannot explicitly create a diffusive flux *from* an Aquifer *to* another pathway, GoldSim actually creates an (invisible) diffusive flux from the Aquifer to the downstream pathway whenever an advective flux is created. When computing the diffusion out of the Aquifer, the concentration in the downstream pathway is treated as zero (which could be a slightly conservative assumption). Note that in most cases, the impact of this diffusive flux will never be noticeable (as it will be dominated by advection).

---

**Read more:** [Understanding How an Aquifer Pathway Works](#) (page 189).

### **Creating and Editing Diffusive Mass Flux Links**

In addition to the **Definition** tab, Cell pathway elements in GoldSim have three additional tabs at the top of their editing dialog: **Inflows**, **Outflows**, and **Diffusive Fluxes**:

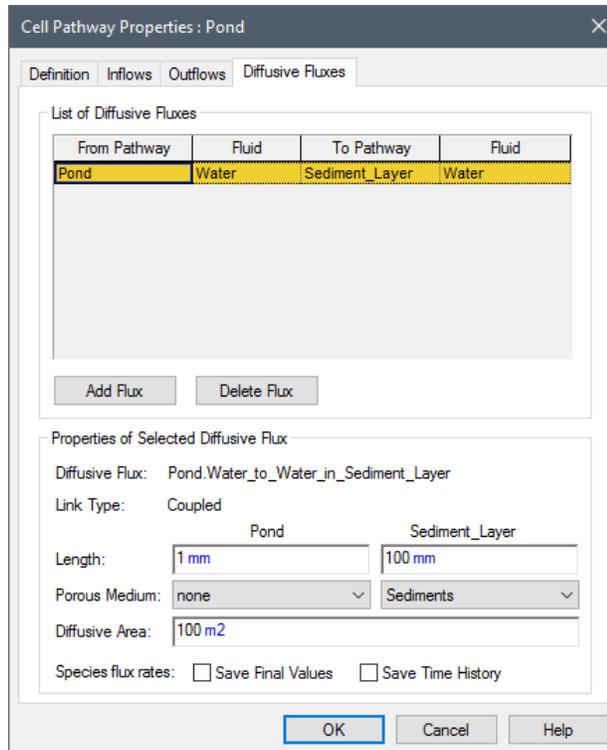


The **Inflows** and **Outflows** tabs are used to create advective and several special purpose mass flux links.

**Read more:** [Creating and Editing Advective Mass Flux Links](#) (page 91).

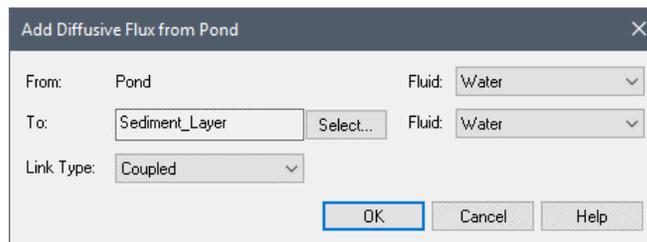
The **Diffusive Fluxes** tab is used to create diffusive flux links involving the current pathway.

The **Diffusive Fluxes** tab is shown below:



To create a new Diffusive Flux (a mass flux link from the current pathway to another pathway), do the following:

1. Double-click on a Cell pathway to display the pathway editing dialog.
2. Click on the **Diffusive Fluxes** tab.
3. Press the **Add Flux** button. This will bring up a browser showing all of the other pathways (or Containers with pathways) in the model.
4. Select the pathway you wish to link to and press **OK**.
5. GoldSim will then display the dialog for selecting the media involved in the mass flux link:



*If you change your mind or have selected the wrong pathway, press the **Select...** button to change the pathway.*

The two fields labeled **Fluid** in this dialog are drop lists containing all of the fluids in the corresponding pathways. (If the mass flux link involves a Pipe, External or Network pathway, the medium involved in the link must be the Reference Fluid, and this will be the only choice in the list.)

The default Link Type for a Diffusive Flux between Cells is Coupled (and, by definition, it cannot be changed). The default Link Type for a

Diffusive Flux to a non-Cell pathway is Normal (and, by definition, it cannot be changed to Coupled).

**Read more:** [Specifying the Link Type for Mass Flux Links](#) (page 118).

Select a fluid in each pathway and press **OK**.

6. You will then be returned to the **Diffusive Fluxes** tab. Move your cursor to the Properties of Selected Diffusive Flux section and enter the Lengths for the two sides of the link. The value must be non-negative. At least one of the lengths must be non-zero.
7. Select the porous medium on each side of the link. The drop-list will include all solids located in the pathway. You do not have to select a porous medium (the default is "none").
8. Specify the Diffusive Area for the link. This must be non-negative.
9. If you wish to save the mass flux Final Values or Time Histories for the link, select one or both of the checkboxes.
10. Press **OK** to close the pathways dialog.



**Note:** If the diffusive flux link involves a non-Cell pathway, the Length and Porous Medium will be grayed out for that side of the connection and set to 0 and none, respectively, since GoldSim assumes that there is no diffusive resistance on the non-Cell side of a diffusive mass flux link.

---

After a diffusive flux is created, you can always change the *properties* of the flux (i.e., the lengths, diffusive areas, porous media, and whether or not results are to be saved) by selecting the diffusive flux in the top of the dialog (by clicking on the appropriate row in the List of Diffusive Fluxes) and editing the properties in the lower section of the dialog (Properties of Selected Diffusive Flux).

The **Diffusive Fluxes** tab only displays the pathway name, and does not indicate where the pathway exists in the model. If, however, you hold your cursor over a pathway in the list, a tooltip displays the full containment path for the pathway.



**Note:** Once a Diffusive Flux is created, you cannot change the fluids which are involved. The only way to change the fluids is to delete the Diffusive Flux and recreate it.

---

A Diffusive Flux is deleted by selecting it in the top of the dialog (by clicking on the appropriate row in the List of Diffusive Fluxes) and pressing the **Delete Flux** button.

When you create a diffusive mass flux link, the link automatically appears in the Diffusive Fluxes tab of both pathways. The properties of the mass flux link can be edited from either location.



**Note:** The Diffusive Fluxes tab is only available for a non-Cell pathway *after* a diffusive link has been made to it. Furthermore, the **Add Flux** button is disabled for non-Cell pathways, preventing you from creating new diffusive flux links (i.e., you can only create new diffusive flux links from Cell pathways).

### Sign Convention for Diffusive Mass Flux Links

Because diffusive mass flux links can be bi-directional, it is important to understand the sign convention used by GoldSim when displaying and using the diffusive mass flux outputs.

Although a diffusive mass flux link can be bi-directional (i.e., mass fluxes can move in either direction along the link), GoldSim always defines one of the two pathways as the "Outflux Pathway" and one of the pathways as the "Influx Pathway". *The pathway from which the link was created via the Diffusive Fluxes tab is identified as the Outflux Pathway for the link.*

Diffusive mass fluxes away from the Outflux Pathway in the link are, by convention, positive, and diffusive mass fluxes toward the Outflux Pathway are negative.

Within the **Diffusive Fluxes** tab for Cell pathways, links in which the cell is the Outflux Pathway are always listed first. Note that because you cannot create a diffusive mass flux link from a non-Cell pathway, non-Cell pathways involved in a diffusive mass flux link can never be an Outflux Pathway.

### Inputs and Outputs Associated with Diffusive Mass Flux Links

When a diffusive mass flux link is created, GoldSim creates several new inputs and outputs on the two linked pathways which subsequently appear in the browser view and interfaces for these pathways.

For the Outflux Pathway in the link:

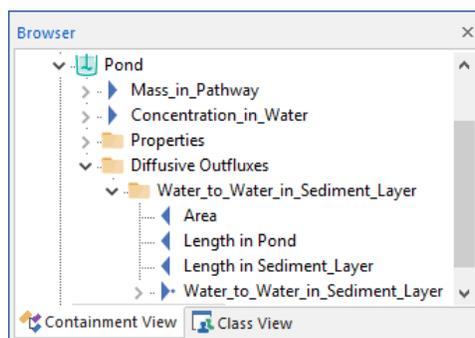
- GoldSim creates a new output named *Medium1\_to\_Medium2\_in\_Path2*, where *Medium1* is the name of the fluid on the Outflux side of the link, *Medium2* is the name of the fluid on the Influx side of the link, and *Path2* is the name of the linked pathway (the Influx Pathway). For example, if Cell1 was linked to Cell2 via a diffusive link in which Water was the fluid on the Outflux side and Air was the fluid on the Influx side, GoldSim would create a new output on the *Cell1* pathway called *Water\_to\_Air\_in\_Cell2*. Like all GoldSim outputs, when the output appears in an expression, the name of the element is included prior to the output name (*Cell1.Water\_to\_Air\_in\_Cell2*). This output represents the mass flux itself, and is a vector by species with dimension of mass/time.



**Note:** Although this output is referred to as a "flux", it technically is a mass rate, not a flux (since fluxes have dimensions of mass/time/area). The term "flux" is used here for convenience.

- GoldSim creates two new inputs named *Length in Path1* and *Length in Path2*, where Path1 is the Outflux pathway, and Path2 is the Influx pathway. These are the thicknesses of the diffusive layer on either side of the link.
- GoldSim creates an additional new input named *Area*. This is the diffusive area for the link.

These new items are organized under a "folder" within the browser view of the element called Diffusive Outfluxes:

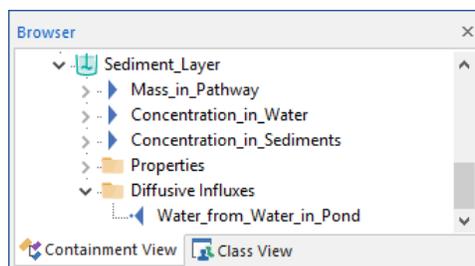


Each diffusive outflux has a separate sub-folder.

For the Influx Pathway in the link:

- GoldSim creates a new input named *Medium2\_from\_Medium1\_in\_Path1*, where *Medium1* is the name of the fluid on the Outflux side of the link, *Medium2* is the name of the fluid on the Influx side of the link, and *Path1* is the name of the linked pathway (the Outflux Pathway). For example, if Cell1 was linked to Cell2 via a diffusive link in which Water was the fluid on the Outflux side and Air was the fluid on the Influx side, GoldSim would create a new input on the Cell2 pathway (the Influx Pathway) called *Air\_from\_Water\_in\_Cell1*.

This item is placed in a Diffusive Influxes "folder" within the browser view of the element:



These new items in the browser views of the pathways are useful because they can be used in conjunction with the Link Cursor to create links. For example, rather than editing the diffusive area in the link using the editing dialog, you could create a link to *Area* using the Link Cursor. Similarly, you could link the mass flux output itself into an Expression element, a Sum element or an Extrema element.

**Read more:** [Manipulating Pathway Outputs](#) (page 253).



**Note:** If you create multiple diffusive fluxes between the same two Cells, GoldSim will append the letter “c” and a number to the end of the input and output names. For example, if a second diffusive flux was added from Cell1 to Cell2, the output on Cell1 would be named “Water\_to\_Air\_in\_Cell2c2” and the input on the Cell2 would be “Air\_from\_Water\_in\_Cell1c2”.

## Understanding Direct Transfer Mass Flux Links

Direct transfer mass flux links are used to transport mass directly from one pathway to another via a mechanism that cannot be appropriately represented as either advection or diffusion. They are defined by specifying a fractional rate at which mass is being moved from one pathway to another. Hence, a direct transfer mass flux is computed as the mass of the species in the pathway multiplied by a fractional transfer rate:

$$\text{Direct Transfer Mass Flux} = \text{Cell Mass} * \text{Transfer Rate}$$

The Transfer Rate has dimensions of inverse time. The Transfer Rate is specified as a vector by species, which allows the Transfer Rate to be species-specific.

As an example of how you might apply a direct transfer mass flux link, consider the following. Suppose that you were simulating the transfer of mass from soil to a plant. You want to represent the kinetics of the transfer process (i.e., you do not want to assume immediate equilibrium). The transfer rate is first order (i.e., proportional to the mass of species in the soil), but cannot be adequately represented as advection (no fluid is moving between the soil and the plant) or diffusion (for example, perhaps the transfer rate is not a function of the concentration of the species in the plant). You could use a direct transfer mass flux link to represent the kinetics in this case.

## Creating and Editing Direct Transfer Mass Flux Links

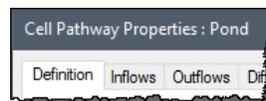
To create a direct transfer mass flux link between two pathways in GoldSim, you must specify a single input:

- The fractional transfer rate. This is specified in terms of inverse time and must be a vector (since the transfer rate can be different for each species). The items of the vector must be non-negative.

Direct transfer mass fluxes can only originate *from* a Cell pathway, although they can be sent *to* any kind of pathway.

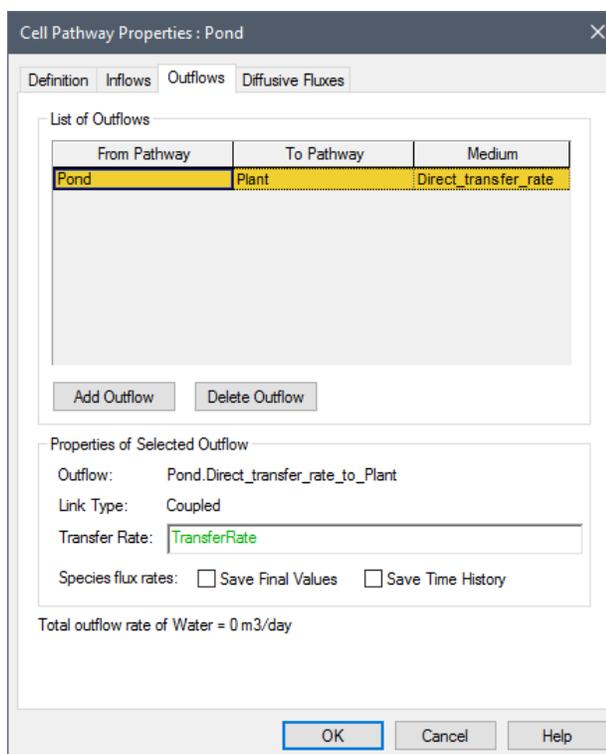
GoldSim provides two ways to create a direct transfer flux link between two pathways:

- By using the **Outflows** tab on the pathway editing dialog; and
- By using the **Inflows** tab on the pathways editing dialog.



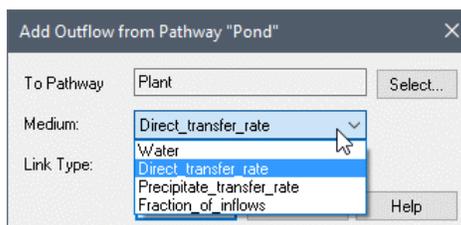
The **Outflows** tab is used to create direct transfer flux links *from* the current pathway *to* other pathways in the model. The **Inflows** tab is used to create direct transfer flux links *to* the current pathway *from* other pathways in the model.

The two dialogs are almost identical in appearance. The **Outflows** tab (with a direct transfer mass flux link) is shown below:



To create a new Outflow (a mass flux link from the current pathway to another pathway), do the following:

1. Double-click on a pathway to display the pathway editing dialog.
2. Click on the **Outflow** tab.
3. Press the **Add Outflow** button. This will bring up a browser showing all of the other pathways (or Containers with pathways) in the model.
4. Select the pathway you wish to link to and press **OK**.
5. GoldSim will then display a dialog for selecting the medium involved in the mass flux link:



*If you change your mind or have selected the wrong pathway, press the **Select...** button to change the pathway.*

The second field in this dialog is a drop list containing the Reference Fluid in the Outflow ("from") pathway, as well any other media that the two pathways have in common. The Medium drop list will also include several other options, including "Direct transfer rate".

The third field in this dialog specifies the Link Type. If you are connecting two Cells, this will default to Coupled. If the link involves any other type of pathway, it will default to Normal. In most cases, you will not need to change the field and can accept the default.

**Read more:** [Specifying the Link Type for Mass Flux Links](#) (page 118).

Select “Direct transfer rate” for the Medium (and select a Link Type) and then press **OK**.

- You will then be returned to the **Outflows** tab. Move your cursor to the Properties of Selected Outflow section and enter the **Transfer Rate** for the link. In this case, this must be a vector by species with dimensions of inverse time, representing the fractional transfer rates for all of the species.



**Note:** The fraction transfer rates for all the species must be non-negative.

---

- If you wish to save the mass flux Final Values or Time Histories for the link, select one or both of the checkboxes.
- Press **OK** to close the pathways dialog.

After an outflow is created, you can always change the *properties* of the outflow (i.e., the transfer rate and whether or not results are to be saved) by selecting the outflow in the top of the dialog (by clicking on the appropriate row in the List of Outflows) and editing the properties in the lower section of the dialog (Properties of Selected Outflow).

The **Inflows** and **Outflows** tab only displays the pathway name, and does not indicate where the pathway exists in the model. If, however, you hold your cursor over a pathway in the list, a tooltip displays the full containment path for the pathway.



**Note:** A direct transfer mass flux link can only be created as an Outflow of a Cell pathway. Any kind of pathway, however, can have a direct transfer mass flux link as an Inflow (i.e., it can receive the mass flux). That is, you can transport mass via a direct transfer mass flux link only *from* Cells but *to* any other kind of pathway.

---

An outflow is deleted by selecting the outflow in the top of the dialog (by clicking on the appropriate row in the List of Outflows) and pressing the **Delete Outflow** button.

The **Inflows** tab can be used to create direct transfer mass flux links *to* the current Cell pathway *from* other Cell pathways in the model. The manner in which inflows are created, edited and deleted is identical to that for outflows, and the two tabs are essentially identical in appearance.

Note that when you create a mass flux link using the **Outflows** tab of one pathway, the link automatically appears in the **Inflows** tab of the linked pathway. The properties of the mass flux link can be edited from either location.

When a direct transfer mass flux link is created, GoldSim creates several new inputs and outputs on the two linked pathways which subsequently appear in the browser view and interfaces for these pathways.

On the "from" or "outflow" pathway (the pathway from which the mass is flowing):

### **Inputs and Outputs Associated with Direct Transfer Mass Flux Links**

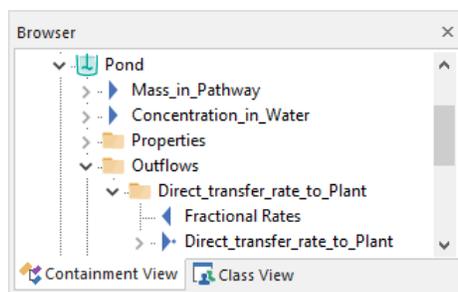
- GoldSim creates a new output named *Direct\_transfer\_rate\_to\_Path2*, where *Path2* is the name of the linked pathway (toward which the mass is flowing). For example, if the Outflow pathway was named *Pond* and the Inflow pathway was named *Plant*, GoldSim would create a new output on the *Pond* pathway called *Direct\_transfer\_rate\_to\_Plant*. Like all GoldSim outputs, when the output appears in an expression, the name of the element is included prior to the output name (*Pond.Direct\_transfer\_rate\_to\_Plant*). This output represents the mass flux itself, and is a vector by species with dimension of mass/time.



**Note:** Although this output is referred to as a “flux”, it technically is a mass rate, not a flux (since fluxes have dimensions of mass/time/area). The term “flux” is used here for convenience.

- GoldSim creates a new input named *Fractional Rates*. This is the transfer rate in the link. It has dimensions of inverse time and is a vector by species.

These new items are organized under a "folder" within the browser view of the element called Outflows:



Each outflow has a separate sub-folder.

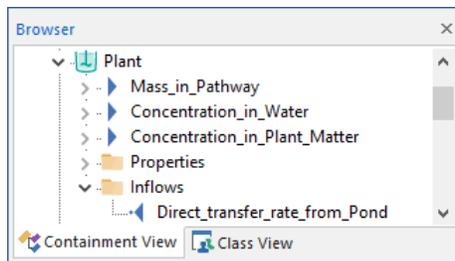
On the "to" or "inflow" pathway (the pathway to which the mass is flowing):

- GoldSim creates a new input named *Direct\_transfer\_from\_Path1*, where *Path1* is the name of the linked pathway (from which the mass is flowing). For example, if the Outflow pathway was named *Pond* and the Inflow pathway was named *Plant*, GoldSim would create a new input on the *Plant* pathway called *Direct\_transfer\_rate\_from\_Pond*. This input represents the mass flux itself, and is a vector by species with dimension of mass/time.



**Note:** Although this output is referred to as a “flux”, it technically is a mass rate, not a flux (since fluxes have dimensions of mass/time/area). The term “flux” is used here for convenience.

This new item is organized under a "folder" within the browser view of the element called Inflows:



**Note:** If you create multiple direct transfer fluxes between the same two Cells, GoldSim will append the letter “c” and a number to the end of the input and output names. For example, if a second direct transfer flux was added from the *Pond* Cell to the *Plant* Cell, the output on the *Pond* Cell would be named “Direct\_transfer\_rate\_to\_Plantc2” and the input on the *Plant* Cell would be “Direct\_transfer\_rate\_from\_Pondc2”.

### Directionality of Direct Transfer Mass Flux Links

You can create as many direct transfer mass flux links as desired in order to build your pathway network. There is, however, one limitation that you must keep in mind regarding the use of direct transfer mass flux links: *Direct transfer mass flux links are uni-directional*. That is, mass can only flow in one direction (negative transfer rates are not allowed). If you wish to simulate a reversal of the transfer direction, you must create two separate direct transfer flux links to represent this (one flowing in one direction, and the other flowing in the other, with the transfer rates defined using expressions which ensure that they are never negative).

### Understanding Precipitate Removal Mass Flux Links

Precipitate removal mass flux links are used to transport precipitated mass directly from one pathway to another. Mass can precipitate in a Cell if solubility limits have been defined for the species in the fluid within the Cell.

**Read more:** [Simulating Solubility Limits in Cells](#) (page 159).

They are defined by specifying a fractional rate at which the precipitated mass is being moved from one pathway to another. Hence, a precipitate removal mass flux is computed as the precipitated mass of the species in the pathway multiplied by a fractional transfer rate:

$$\text{Precipitate Removal Mass Flux} = \text{Precipitated Cell Mass} * \text{Transfer Rate}$$

The Transfer Rate has dimensions of inverse time. The Transfer Rate is specified as a scalar. That is, all precipitate species are transferred at the same rate.

In most applications, the Transfer Rate will simply be input either as a large number (such that any precipitated mass is immediately removed) or a function that alternates between 0 and a large number (such that any precipitated mass is periodically removed, and allowed to accumulate between removals).

Note that in most cases, in order to use a Precipitate removal mass flux link you will need to specify a local solubility (a solubility that varies depending where you are in the model).

**Read more:** [Defining Spatially Variable Media Properties](#) (page 295).

As an example of how you might apply a precipitate removal mass flux link, consider the following. Suppose that you were simulating a process in which a particular metal was precipitated out of solution within a tank. Once a month, you removed the precipitate from the tank. You could use a precipitate removal

### Creating and Editing Precipitate Removal Mass Flux Links

transfer flux link to represent the kinetics in this case. You would create a link to a Sink Cell (where the precipitate is collected), and the transfer rate would be increased to a large number once per month (e.g., for 1 day), which would have the effect of "cleaning out" the tank of any precipitate. For the rest of the simulation, the transfer rate would be zero (and precipitate would collect in the tank).

To create a precipitate removal mass flux link between two pathways in GoldSim, you must specify a single input:

- The fractional transfer rate. This is specified in terms of inverse time and must be a scalar (the transfer rate is assumed to be identical for each species). The transfer rate must be non-negative.

Precipitate removal mass fluxes can only originate *from* a Cell pathway, although they can be sent *to* any kind of pathway.



**Note:** Once the mass is transferred to another pathway, it will not necessarily remain precipitated, depending on properties of the pathway. If it is transferred to a Pipe pathway, for example, all the mass will immediately be mobilized (i.e., assumed to be dissolved).

---

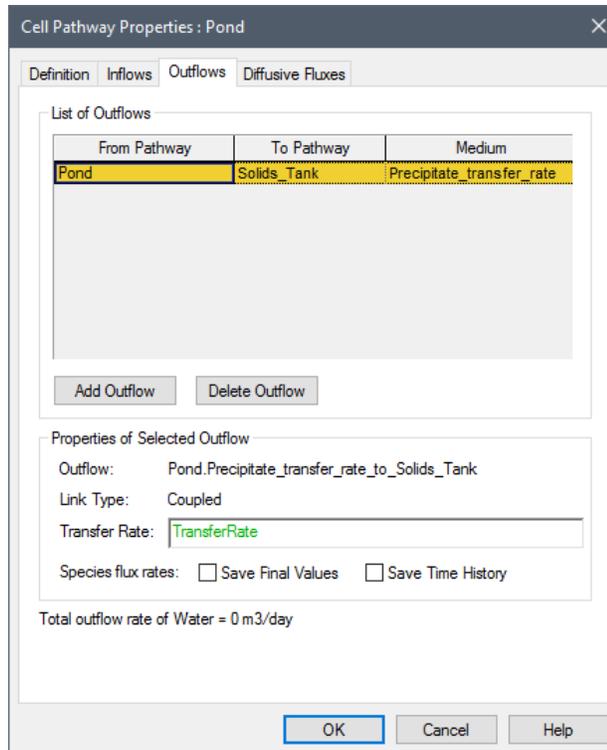
GoldSim provides two ways to create a precipitate removal flux link between two pathways:

- By using the **Outflows** tab on the pathway editing dialog; and
- By using the **Inflows** tab on the pathways editing dialog.



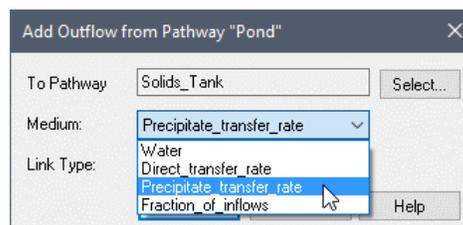
The **Outflows** tab is used to create precipitate removal flux links *from* the current pathway *to* other pathways in the model. The **Inflows** tab is used to create precipitate removal flux links *to* the current pathway *from* other pathways in the model.

The two dialogs are almost identical in appearance. The **Outflows** tab (with a precipitate removal mass flux link) is shown below:



To create a new Outflow (a mass flux link from the current pathway to another pathway), do the following:

1. Double-click on a pathway to display the pathway editing dialog.
2. Click on the **Outflow** tab.
3. Press the **Add Outflow** button. This will bring up a browser showing all of the other pathways (or Containers with pathways) in the model.
4. Select the pathway you wish to link to and press **OK**.
5. GoldSim will then display a dialog for selecting the medium involved in the mass flux link:



*If you change your mind or have selected the wrong pathway, press the **Select...** button to change the pathway.*

The second field in this dialog is a drop list containing the Reference Fluid in the Outflow ("from") pathway, as well any other media that the two pathways have in common. The Medium drop list will also include several other options, including "Precipitate transfer rate".

The third field in this dialog specifies the Link Type. If you are connecting two Cells, this will default to Coupled. If the link involves any other type of pathway, it will default to Normal. In most cases, you will not need to change the field and can accept the default.

**Read more:** [Specifying the Link Type for Mass Flux Links](#) (page 118).

Select “Precipitate transfer rate” for the Medium (and select a Link Type) and then press **OK**.

6. You will then be returned to the **Outflows** tab. Move your cursor to the Properties of Selected Outflow section and enter the **Transfer Rate** for the link. In this case, this must be a vector by species with dimensions of inverse time, representing the fractional transfer rates for all of the species.



**Note:** The fraction transfer rates for all the species must be non-negative.

---

7. If you wish to save the mass flux Final Values or Time Histories for the link, select one or both of the checkboxes.
8. Press **OK** to close the pathways dialog.

After an outflow is created, you can always change the *properties* of the outflow (i.e., the transfer rate and whether or not results are to be saved) by selecting the outflow in the top of the dialog (by clicking on the appropriate row in the List of Outflows) and editing the properties in the lower section of the dialog (Properties of Selected Outflow).

The **Inflows** and **Outflows** tab only displays the pathway name, and does not indicate where the pathway exists in the model. If, however, you hold your cursor over a pathway in the list, a tooltip displays the full containment path for the pathway.



**Note:** A precipitate removal mass flux link can only be created as an Outflow of a Cell pathway. Any kind of pathway, however, can have a precipitate removal mass flux link as an Inflow (i.e., it can receive the mass flux). That is, you can transport mass via a precipitate removal mass flux link only *from* Cells but *to* any other kind of pathway.

---

An outflow is deleted by selecting the outflow in the top of the dialog (by clicking on the appropriate row in the List of Outflows) and pressing the **Delete Outflow** button.

The **Inflows** tab can be used to create precipitate removal mass flux links *to* the current Cell pathway *from* other Cell pathways in the model. The manner in which inflows are created, edited and deleted is identical to that for outflows, and the two tabs are essentially identical in appearance.

Note that when you create a mass flux link using the **Outflows** tab of one pathway, the link automatically appears in the **Inflows** tab of the linked pathway. The properties of the mass flux link can be edited from either location.

When a precipitate removal mass flux link is created, GoldSim creates several new inputs and outputs on the two linked pathways which subsequently appear in the browser view and interfaces for these pathways.

On the "from" or "outflow" pathway (the pathway from which the mass is flowing):

### **Inputs and Outputs Associated with Precipitate Removal Mass Flux Links**

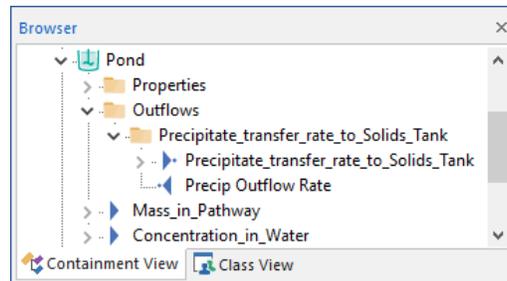
- GoldSim creates a new output named *Precipitate\_transfer\_rate\_to\_Path2*, where *Path2* is the name of the linked pathway (toward which the mass is flowing). For example, if the Outflow pathway was named *Pond* and the Inflow pathway was named *Solids\_Tank*, GoldSim would create a new output on the *Pond* pathway called *Precipitate\_transfer\_rate\_to\_Solids\_Tank*. Like all GoldSim outputs, when the output appears in an expression, the name of the element is included prior to the output name (*Pond.Precipitate\_transfer\_rate\_to\_Solids*). This output represents the mass flux itself, and is a vector by species with dimension of mass/time.



**Note:** Although this output is referred to as a “flux”, it technically is a mass rate, not a flux (since fluxes have dimensions of mass/time/area). The term “flux” is used here for convenience.

- GoldSim creates a new input named *Precip Outflow Rate*. This is the transfer rate in the link. It has dimensions of inverse time and is a scalar.

These new items are organized under a "folder" within the browser view of the element called Outflows:



Each outflow has a separate sub-folder.



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

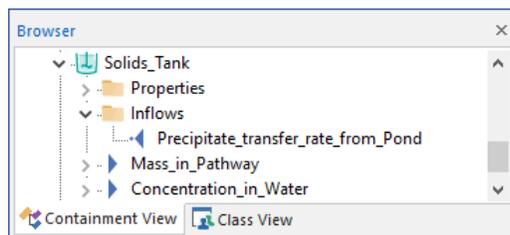
On the "to" or "inflow" pathway (the pathway to which the mass is flowing):

- GoldSim creates a new input named *Direct\_transfer\_from\_Path1*, where *Path1* is the name of the linked pathway (from which the mass is flowing). For example, if the Outflow pathway was named *Pond* and the Inflow pathway was named *Solids\_Tank*, GoldSim would create a new input on the *Solids\_Tank* pathway called *Precipitate\_transfer\_rate\_from\_Pond*. This input represents the mass flux itself, and is a vector by species with dimension of mass/time.



**Note:** Although this output is referred to as a “flux”, it technically is a mass rate, not a flux (since fluxes have dimensions of mass/time/area). The term “flux” is used here for convenience.

This new item is organized under a "folder" within the browser view of the element called Inflows:



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

**Note:** If you create multiple precipitate removal mass transfer fluxes between the same two Cells, GoldSim will append the letter "c" and a number to the end of the input and output names. For example, if a second direct transfer flux was added from *Pond* Cell to the *Solids\_Tank* Cell, the output on the *Pond* Cell would be named "Precipitate\_transfer\_rate\_to\_Solids)Tankc2" and the input on the *Solids\_Tank* Cell would be "Precipitate\_transfer\_rate\_from\_Pondc2".

### Directionality of Precipitate Removal Mass Flux Links

You can create as many precipitate removal mass flux links as desired in order to build your pathway network. There is, however, one limitation that you must keep in mind regarding the use of these mass flux links: *Precipitate removal mass flux links are uni-directional*. That is, mass can only flow in one direction (negative transfer rates are not allowed). If you wish to simulate a reversal of the transfer direction, you must create two separate precipitate removal flux links to represent this (one flowing in one direction, and the other flowing in the other, with the transfer rates defined using expressions which ensure that they are never negative).

### Understanding Fraction of Inflows (Treatment) Mass Flux Links

Fraction of inflows mass flux links (hereafter referred to as treatment mass flux links) are used to provide a mechanism for treating or removing a fraction of the amount of mass entering a Cell. They are defined by specifying a fraction of the mass entering the pathway which is removed. Hence, a treatment mass flux is computed as the mass rate of inflow of the species entering the pathway multiplied by a fraction:

$$\text{Treatment Mass Flux} = \text{Cell Mass Inflow Rate} * \text{Fraction}$$

The Fraction is dimensionless, and must be greater than or equal to 0 and less than or equal to 1. The Fraction is specified as a vector by species, which allows the Fraction to be species-specific.

As an example of how you might apply a treatment mass flux link, consider the following. Suppose that you were simulating a tank that chemically removed a certain fraction of each species as it entered the tank. You could use a treatment flux link to represent the kinetics in this case. You would specify the removal fraction (i.e., the treatment efficiency) for each species, and create a link to a Sink cell where all of the removed (treated) mass is accumulated.



**Warning:** Treatment mass flux links only act on mass fluxes that are entering from outside the Cell net to which the Cell belongs. Hence, in order to filter incoming fluxes, the incoming mass fluxes must be specified as Normal or Previous-Value (as opposed to Coupled) flux links (or must be specified as direct inflows via the Cell Inventory field). Coupled influges are not impacted by treatment mass flux links. If a Cell that has an outgoing treatment mass flux links has no incoming Normal or Previous-Value links or influges through a specified Cell Inventory, GoldSim will display a fatal error message.

## Creating and Editing Treatment Mass Flux Links

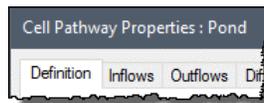
To create a treatment mass flux link between two pathways in GoldSim, you must specify a single input:

- The fractional removal rate (the treatment efficiency). This is dimensionless and must be a vector (since the fraction can be different for each species). The items of the vector must be greater than or equal to 0 and less than or equal to 1.

Treatment mass fluxes can only originate *from* a Cell pathway, although they can be sent *to* any kind of pathway.

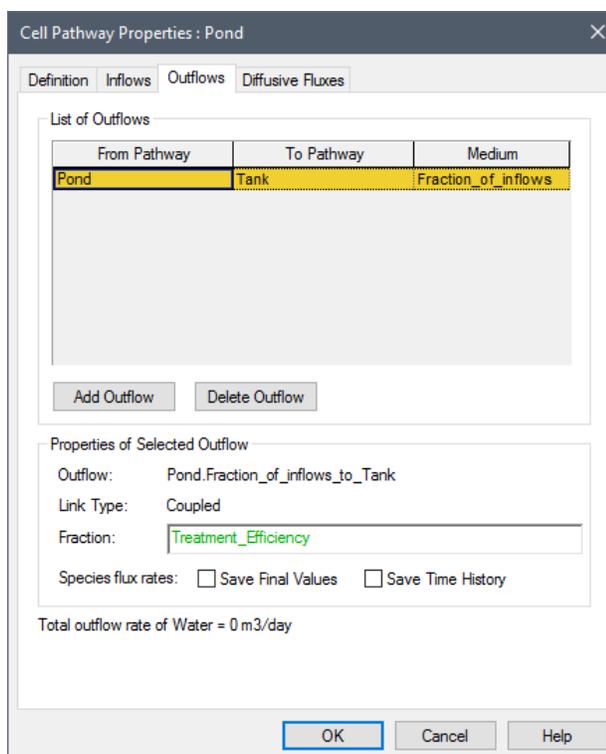
GoldSim provides two ways to create a treatment flux link between two pathways:

- By using the **Outflows** tab on the pathway editing dialog; and
- By using the **Inflows** tab on the pathways editing dialog.



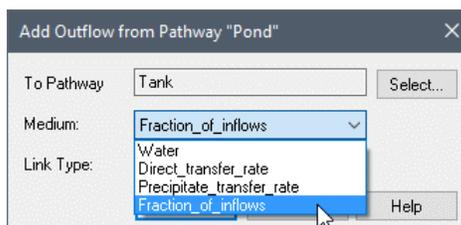
The **Outflows** tab is used to create treatment flux links *from* the current pathway *to* other pathways in the model. The **Inflows** tab is used to create treatment flux links *to* the current pathway *from* other pathways in the model.

The two dialogs are almost identical in appearance. The **Outflows** tab (with a treatment mass flux link) is shown below:



To create a new Outflow (a mass flux link from the current pathway to another pathway), do the following:

1. Double-click on a pathway to display the pathway editing dialog.
2. Click on the **Outflow** tab.
3. Press the **Add Outflow** button. This will bring up a browser showing all of the other pathways (or Containers with pathways) in the model.
4. Select the pathway you wish to link to and press **OK**.
5. GoldSim will then display a dialog for selecting the medium involved in the mass flux link:



*If you change your mind or have selected the wrong pathway, press the **Select...** button to change the pathway.*

The second field in this dialog is a drop list containing the Reference Fluid in the Outflow ("from") pathway, as well as any other media that the two pathways have in common. The Medium drop list will also include "Fraction of inflows".

The third field in this dialog specifies the Link Type. If you are connecting two Cells, this will default to Coupled. If the link involves any other type of pathway, it will default to Normal. In most cases, you will not need to change the field and can accept the default.

**Read more:** [Specifying the Link Type for Mass Flux Links](#) (page 118).

Select “Fraction of inflows” for the Medium (and select a Link Type) and then press **OK**.

- You will then be returned to the **Outflows** tab. Move your cursor to the Properties of Selected Outflow section and enter the **Fraction** for the link. In this case, this must be a dimensionless vector by species, representing the removal fractions for all of the species.



**Note:** The fractions for all the species must be greater than or equal to 0 and less than or equal to 1.

---

- If you wish to save the mass flux Final Values or Time Histories for the link, select one or both of the checkboxes.
- Press **OK** to close the pathways dialog.



**Note:** A Cell can only have a single treatment mass flux link. GoldSim will not allow you to create more than one.

---

After an outflow is created, you can always change the *properties* of the outflow (i.e., the fraction and whether or not results are to be saved) by selecting the outflow in the top of the dialog (by clicking on the appropriate row in the List of Outflows) and editing the properties in the lower section of the dialog (Properties of Selected Outflow).

The **Inflows** and **Outflows** tab only displays the pathway name, and does not indicate where the pathway exists in the model. If, however, you hold your cursor over a pathway in the list, a tooltip displays the full containment path for the pathway.



**Note:** A treatment mass flux link can only be created as an Outflow of a Cell pathway. Any kind of pathway, however, can have a treatment mass flux link as an Inflow (i.e., it can receive the mass flux). That is, you can transport mass via a treatment mass flux link only *from* Cells but *to* any other kind of pathway.

---

An outflow is deleted by selecting the outflow in the top of the dialog (by clicking on the appropriate row in the List of Outflows) and pressing the **Delete Outflow** button.

The **Inflows** tab can be used to create treatment mass flux links *to* the current Cell pathway *from* other Cell pathways in the model. The manner in which inflows are created, edited and deleted is identical to that for outflows, and the two tabs are essentially identical in appearance.

Note that when you create a mass flux link using the **Outflows** tab of one pathway, the link automatically appears in the **Inflows** tab of the linked pathway. The properties of the mass flux link can be edited from either location.

### **How Treatment Mass Flux Links Work**

When you create a treatment mass flux link from a Cell, this is how it is implemented within GoldSim:

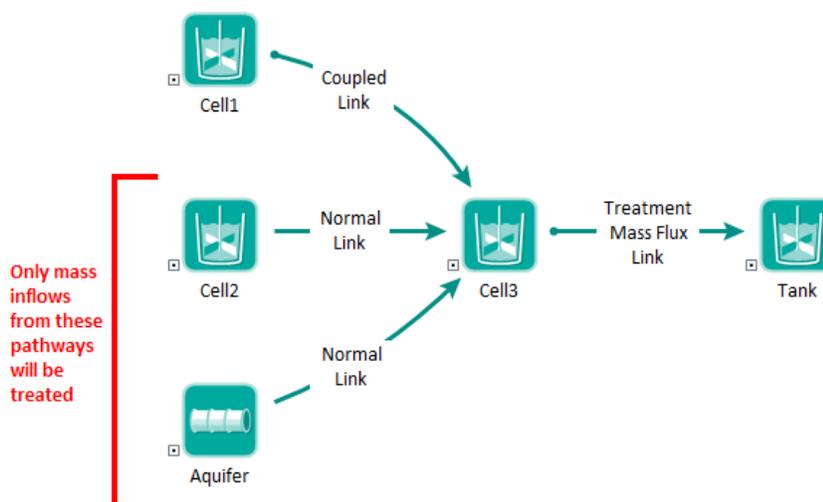
1. GoldSim adds all of the non-coupled influxes to the Cell (fluxes whose Link Type is Normal or Previous-value), along with any external fluxes specified via the Cumulative Input field.



**Warning:** Mass present in a Cell at the beginning of a simulation (i.e., initial conditions) are not treated. That is, mass initially present in the Cell cannot be removed using a treatment flux link.

2. The Fraction defined for the treatment mass flux link is multiplied by the summed influxes. The product of this is then immediately transferred via the treatment mass flux link out of the Cell.
3. All other Cell calculations are then carried out on the remaining mass in the Cell (e.g., other flux links, solubility and sorption calculations).

It is worth reiterating here that treatment mass flux links only act on mass fluxes that are entering from outside the Cell net to which the Cell belongs (i.e., they do not act on any mass entering via Coupled links). Hence, in order to treat incoming fluxes, you must first specify them as Normal (as opposed to Coupled) flux links (or must be specified as direct inputs via the Cumulative Inputs field). Coupled influxes will not be impacted:



Coupled links can be identified by the small circle at the beginning of the influence.

**Read more:** [Specifying the Link Type for Mass Flux Links](#) (page 118).

### Inputs and Outputs Associated with Treatment Mass Flux Links

When a treatment mass flux link is created, GoldSim creates several new inputs and outputs on the two linked pathways which subsequently appear in the browser view and interfaces for these pathways.

On the "from" or "outflow" pathway (the pathway from which the mass is flowing):

- GoldSim creates a new output named *Fraction\_of\_inflows\_to\_Path2*, where *Path2* is the name of the linked pathway (toward which the mass is flowing). For example, if the Outflow pathway was named *Pond* and the Inflow pathway was named *Tank*, GoldSim would create a new output on the *Pond* pathway called *Fraction\_of\_inflows\_to\_Tank*. Like all GoldSim outputs, when the output appears in an expression, the name of the element is included prior to the output name (*Pond*).

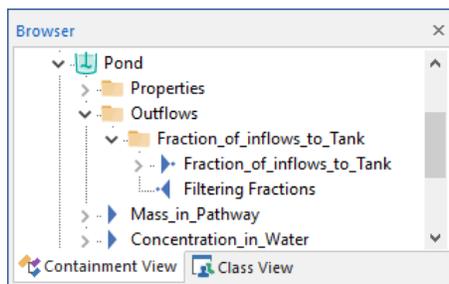
*Fraction\_of\_inflows\_to\_Tank*). This output represents the mass flux itself, and is a vector by species with dimension of mass/time.



**Note:** Although this output is referred to as a “flux”, it technically is a mass rate, not a flux (since fluxes have dimensions of mass/time/area). The term “flux” is used here for convenience.

- GoldSim creates a new input named *Filtering Fractions*. These are the actual fractions. It is dimensionless and is a vector by species.

These new items are organized under a "folder" within the browser view of the element called Outflows:



Each outflow has a separate sub-folder.



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

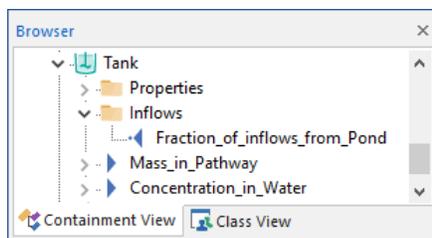
On the "to" or "inflow" pathway (the pathway to which the mass is flowing):

- GoldSim creates a new input named *Direct\_transfer\_from\_Path1*, where *Path1* is the name of the linked pathway (from which the mass is flowing). For example, if the Outflow pathway was named *Pond* and the Inflow pathway was named *Tank*, GoldSim would create a new input on the *Sink* pathway called *Fraction\_of\_inflows\_from\_Pond*. This input represents the mass flux itself, and is a vector by species with dimension of mass/time.



**Note:** Although this output is referred to as a “flux”, it technically is a mass rate, not a flux (since fluxes have dimensions of mass/time/area). The term “flux” is used here for convenience.

This new item is organized under a "folder" within the browser view of the element called Inflows:



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

### Directionality of Treatment Mass Flux Links

You can create as many treatment mass flux links as desired in order to build your pathway network. There is, however, one limitation that you must keep in mind regarding the use of treatment mass flux links: *Treatment mass flux links are uni-directional*. That is, mass can only flow in one direction (negative transfer rates are not allowed).

### Specifying the Link Type for Mass Flux Links

There are three types of mass flux links in GoldSim. A mass flux link between two pathways can be defined as a **normal link**, a **previous value link**, or a **coupled link**. When you create a mass flux link, a drop list is available to allow you to select the type of link.

- In a coupled link, the equations for the pathways and their fluxes are solved simultaneously (since they are solved as a system of coupled differential equations as part of a **cell net**). Only links between Cells can be coupled. The influence representing a coupled link takes on a special shape:



*Coupled links can be identified by the small circle at the beginning of the influence.*

**Read more:** [Understanding Cell Nets](#) (page 165).

- In a normal link, at each timestep the “upstream” pathway’s output is computed and then applied to the “downstream” pathway. That is, the mass is propagated asynchronously (i.e., the “upstream” pathway is solved first, followed by the “downstream” one).
- In a previous value link, at each timestep the “upstream” pathway’s output from the **previous timestep** is applied to the “downstream” pathway. So, like a normal link, the mass is propagated asynchronously (but with a timestep delay).



**Note:** Although normal and previous value links are not “coupled”, numerically they are still represented implicitly (rather than explicitly). They are simply propagated asynchronously.

By default, mass flux links between Cells are coupled links.

Mass flux links to or from other types of pathways are defaulted to normal links (and cannot be coupled). Note that only flux links between Cells can be coupled links. Diffusive mass flux links between Cells *must* be coupled (i.e., the other options are not available in this case).



**Note:** For advection, solving pathway equations asynchronously (rather than in a coupled manner) is mathematically feasible, since the advective mass flux from one pathway to another is only a function of the concentration in the upstream pathway (i.e., it is not necessary to reference the downstream pathway to compute the mass flux). Although we can model advection by solving the Cells asynchronously (rather than in a coupled manner), doing so can in fact reduce the accuracy of the solution. This is related to the fact that GoldSim effectively subdivides the computational timestep (into *fractional timesteps*) when solving a cell net to improve accuracy (when the Medium or High Precision setting is selected). “Breaking” a Cell Net and computing fluxes between cells asynchronously effectively reduces the effectiveness of the fractional timesteps, and hence reduces the accuracy somewhat (in the same manner that using the Low Precision setting does). For most systems, using Normal links in a model in several locations (as opposed to throughout the entire model) would be unlikely to affect the results significantly. Using Previous-value links would introduce a more noticeable error (effectively delaying results by a timestep for each Previous-value link in the sequence of Cells). Again, however, for most realistic situations, using Previous-value links a model in several locations is also not likely to affect the results significantly.

You will rarely, if ever, need to change the link type from the default.

There are some special cases, however, when it may be necessary to modify the type of link connecting pathways:

- *Changing a coupled or normal mass flux link to a previous value mass flux link:* This may be necessary if you are building a looping pathway network.

**Read more:** [Simulating Looping Pathway Networks](#) (page 256).

- *Changing a coupled mass flux link to a normal mass flux link:* This change is necessary if you wish to “filter” an incoming flux (using a treatment flux link).

**Read more:** [Understanding Fraction of Inflows \(Treatment\) Mass Flux Links](#) (page 112).

- *Changing a coupled mass flux link to a normal mass flux link:* The computational effort to solve the coupled equations of a large number of Cells increases rapidly (i.e., not linearly) with the number of Cells. In most models, this is not a problem, but for extremely large models (hundreds of Cells), it may be worthwhile to break a very large set of coupled Cells (a Cell Net) into several smaller Cell Nets (by using a Normal link).

## Using Cell Pathways

Cell pathways are the most versatile of the four GoldSim Contaminant Transport Module pathways. In many cases, this may be the only pathway type that you will need to build your model. Cell pathways are intended to represent discrete,

## Features and Capabilities of Cells

well-mixed environmental compartments or "mixing cells" within the environmental system that you are simulating.

A Cell pathway is mathematically equivalent to a mixing cell, and can explicitly represent the following processes:

- **Partitioning.** You can assign multiple fluid or solid media (e.g., water, oil, rust, soil) to a Cell, and specify partition coefficients between the various media. Contaminant mass is instantaneously and completely mixed and equilibrated throughout the Cell, and contaminants are partitioned between the various media based on the partition coefficients and masses/volumes of the various media present.
- **Solubility constraints.** You can assign solubility limits for the contaminants in the Reference Fluid (typically water) present in the Cell. The dissolved concentration of the contaminants in the Cell cannot exceed the solubility limit. If you are simulating isotopes of the same element, GoldSim ensures that the sum of the concentrations of all isotopes does not exceed the solubility limit.
- **Mass transport.** You can define the processes and properties controlling the rate at which mass moves between pathways (e.g., from one Cell to another). Both advective and diffusive transport mechanisms can be explicitly represented (using advective and diffusive mass flux links). Other transport mechanisms can also be represented by using direct transfer mass flux links. Solids present in a Cell can be specified to be suspended in the Cell's fluid media, such that the transport of contaminants on suspended particulates (via advection or diffusion) can be explicitly modeled.

When multiple Cells are linked together via advective and diffusive mechanisms, the behavior of the Cell network is mathematically described using a coupled system of differential equations. GoldSim numerically solves the coupled system of equations to compute the contaminant mass present in each Cell (and the mass transfer rates between Cells) as a function of time.

The following sections describe the basic assumptions incorporated into Cell pathways, and how to define and use them in your models. The mathematical and computational details of how Cell pathways are implemented within GoldSim are provided in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

### Cell Pathway Example #1: Partitioning and Decay

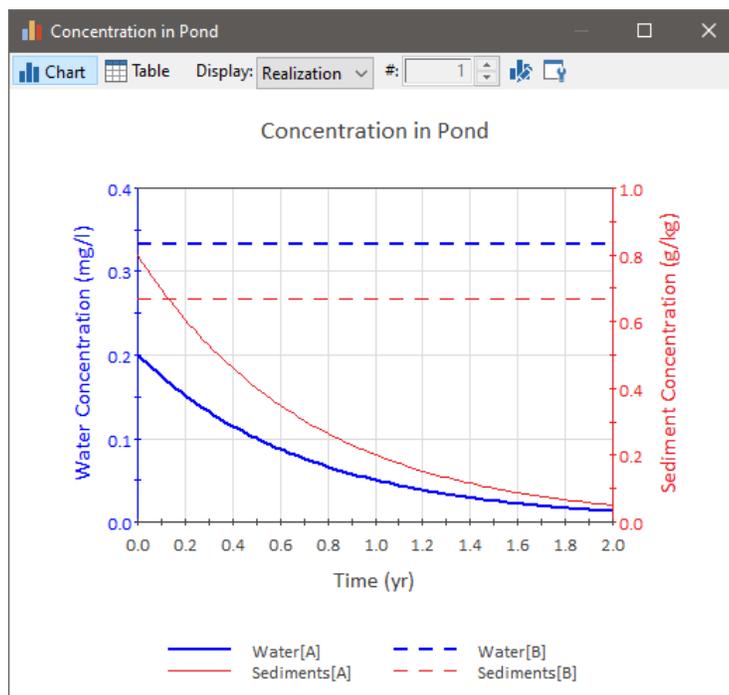
Before describing the details involved in using Cell pathways, it is worthwhile to present a very simple example in order to begin to understand the kinds of problems that can be solved using Cells. This particular example file, Cell1\_PartitioningDecay.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu). This example illustrates how GoldSim simulates partitioning, decay and ingrowth.

Suppose that 10 g of chemicals A and B are released into a small pond. The pond contains two media: Water and Sediments. Chemical A degrades according to a first order reaction, with a half-life of 0.5 years. Both A and B sorb onto the Sediments. This sorption can be quantified by specifying partition coefficients (equal to 4 m<sup>3</sup>/kg for A and 2 m<sup>3</sup>/kg for B). Because the pond is shallow, it is assumed that it is well-mixed, and the Water and Sediments are instantaneously at equilibrium with respect to partitioning of the species. You wish to predict the concentration of the two species in the Water and Sediments in the pond as a function of time.

To simulate this system in GoldSim, you would do the following:

1. Define two species (A and B) and specify their decay properties;
2. Define two media (Water and Sediments) and specify their properties (e.g., the partition coefficients);
3. Define a single Cell pathway to represent the pond;
4. Specify the quantities of Water and Sediment present in the pond Cell;
5. Specify an initial mass of species in the pond Cell; and
6. Specify the simulation settings (i.e., duration and timesteps), and run the model.

The output of this simulation, in the form of time histories of the concentrations of species A and B in the Water and Sediments in the pond, is shown below:



Note that because A decays (and B does not), the concentration of A (in Water and Sediments) decreases, while the concentration of B is constant. Because both species partition onto the Sediments, they are present in both media. The system is assumed to be well-mixed, such that equilibrium is reached immediately. As a result, the ratio of the concentration of A and in Water to that in Sediments is constant (and equal to  $4 \text{ m}^3/\text{kg}$  for A and  $2 \text{ m}^3/\text{kg}$  for B).

A slightly different version of this example (that includes ingrowth, such that A decays to B), Cell1\_PartitioningDecayIngrowth.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

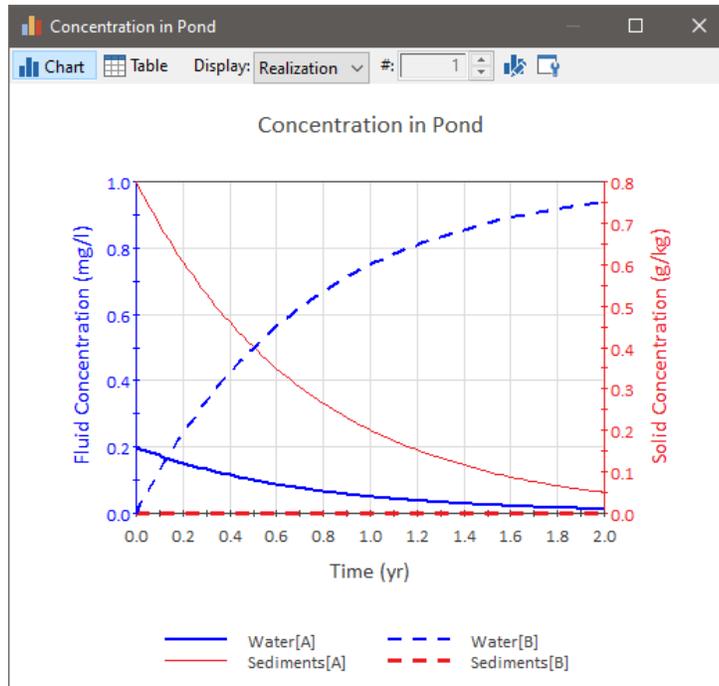


**Note:** Because this example includes ingrowth, it requires the RT Module. If you are using the CT Module, you will not be able to open the file.

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4).

In Cell1\_PartitioningDecayIngrowth.gsm, the model is defined slightly differently than the example with no ingrowth: 1) No B is initially present in the pond; 2) A decays to B; and 3) B does not partition onto Sediments (although A still does).

The output of this simulation, in the form of time histories of the concentrations of species A and B in the Water and Sediments in the pond, is shown below:



Note that because A decays to B, the concentration of A (in Water and Sediments) decreases, while the concentration of B increases. Because A partitions onto the Sediments, it is present in both media (B is not present in Sediments). The system is assumed to be well-mixed, such that equilibrium is reached immediately. As a result, the ratio of the concentration of A and in Water to that in Sediments is constant (and equal to 4 m<sup>3</sup>/kg for A).

Note that in these simple examples, the system is closed (i.e., mass does not enter or leave the pond). Subsequent examples consider mass flux links to and from Cells.

## Defining Basic Cell Properties

The editing dialog for a Cell pathway is shown below:

Cell Pathway Properties : Pond

Definition Inflows Outflows Diffusive Fluxes

Element ID:  Appearance...

Description:

Media in Cell

Medium	Amount	F	H	S
Water	10 m3	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Sediments	10 kg	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Add Medium Delete Medium

Cell Inventory

Initial Inventory

Discrete Changes:

Save Masses in Pathway

Output Precipitated Mass

Final Values  Time History

OK Cancel Help

The primary input that must be defined for a Cell pathway is the quantity of each medium present in the pathway. The Reference Fluid is automatically present in each Cell when it is first created. The number of additional Fluids and Solids that can be added to the Cell is unlimited, but most Cells will typically include no more than one or two additional media.

### Adding and Deleting Cell Media

Media are added to and deleted from a Cell using the **Add Medium** and **Delete Medium** buttons.

To add a new medium:

1. Press the **Add Medium** button to display a browser showing all of the media (and Containers with media) in the model.
2. Select the medium you wish to add to the pathway and press **OK**.
3. GoldSim will add the medium to the list of media in the cell dialog and highlight it (in yellow). Place your cursor in the **Amount** column and specify (as a number or via a link or expression) the quantity of the medium in the pathway. You must specify the quantity in terms of volume for Fluids and mass for Solids.



**Warning:** If the quantity of a medium in a Cell is not constant (and you are running at Medium or High Precision), the concentrations are computed based on an effective amount (a weighted average over the timestep). This can result in errors in the computed concentrations (and hence the mass flux rates) if the quantity is changing rapidly over a timestep. As a general rule, the errors will be insignificant as long as the quantity changes by less than 10% over a timestep. If this is not the case, you should reduce the timestep to ensure that it is.



**Warning:** If the quantity of a medium in a Cell goes completely to zero, some mass will be left behind in the Cell (until media is added to the Cell again). Although this may actually be physically realistic in some cases (e.g., outflow due to evaporation, and hence precipitation of the mass), in other cases it is not. The magnitude of the error can be reduced by reducing the timestep as the Cell approaches being empty.

**Read more:** [Dealing with Changing Media Amounts in a Cell](#) (page 169).



**Note:** A medium that has zero volume (fluids) or mass (solids) cannot have a species concentration. Any mass in the Cell will either partition into other Fluids (if present) or in the absence of other Fluids into which the mass can partition, precipitate out onto any Solids present in the Cell (proportional to the mass of each Solid) even if no solubility limit is specified.

To delete an existing medium:

1. Select the medium you wish to delete by clicking on it in the media list for the cell (the selected medium is highlighted in yellow).
2. Press the **Delete Medium** button.



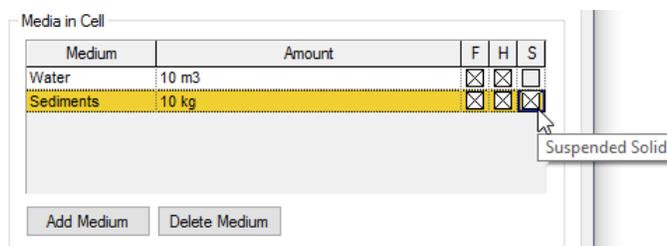
**Note:** GoldSim will warn you if you try to delete a medium that is referenced in a mass flux link for the Cell. In this case, deleting the medium will also delete the mass flux link.

### Defining Suspended Solids in a Cell

When you add a Solid to a Cell, you can specify that the Solid is present in the Cell as suspended particulate matter. The Solid is assumed to be suspended in the first Fluid that precedes it in the list of media for the cell.

To specify that a Solid is suspended:

1. Select the Solid from the list of media in the Cell by clicking on it (the selected Solid will be highlighted in yellow).
2. Check the "Suspended" box (labeled "S") to the immediate right of the specified Solid:



If a Solid is suspended, species mass sorbed to the Solid is transported in any mass flux links involving the Fluid in which the Solid is suspended.

**Read more:** [Advection of Particulates to/from Cells](#) (page 138); [Diffusion of Particulates to/from Cells](#) (page 141).



**Note:** If you wish to specify that only a portion of a Solid is suspended, add the Solid to the media list for the Cell twice (or define two different Solids with the same properties), and only specify that the Solid is suspended in one instance. Similarly, if you wish to specify that the Solid is suspended in multiple fluids in the Cell, add the Solid to the media list multiple times below the appropriate Fluids.



**Note:** Whenever you create a suspended Solid in a Cell, GoldSim creates an additional output for the Cell. In particular, in addition to computing the total concentration of the species in the Fluid in which the solid is suspended, it also computes the dissolved concentration of the species in the Fluid (excluding the contribution from species that are sorbed onto suspended particulates).

**Read more:** [Cell Pathway Outputs](#) (page 133).

### Understanding Partitioning in a Cell

When species mass enters a Cell, it is instantaneously partitioned among the media present in the Cell. The partitioning is controlled by the partition coefficients defined for each species in each medium, and the quantity of each medium present. In particular, *in the absence of solubility limits*, the concentration of species  $i$  in Medium  $x$  is computed by GoldSim as follows:

$$c_{xi} = \left( \frac{K_{xi}}{\sum_{g=1}^{NM} K_{gi} \cdot VM_g} \right) m_i$$

where:

- $c_{xi}$  = concentration of species  $i$  in medium  $x$  in the cell [(M/L<sup>3</sup>) for Fluids or (M/M) for Solids];
- $m_i$  = mass of species  $i$  in the cell [M];
- $K_{xi}$  = partition coefficient between medium  $x$  and Reference Fluid for species  $i$  [(L<sup>3</sup>/L<sup>3</sup>) for Fluids or (L<sup>3</sup>/M) for Solids];
- $K_{gi}$  = partition coefficient between medium  $g$  and Reference Fluid for species  $i$  [(L<sup>3</sup>/L<sup>3</sup>) for Fluids or (L<sup>3</sup>/M) for Solids];
- $VM_g$  = quantity (volume or mass) of medium  $g$  in the cell [L<sup>3</sup> for Fluids or M for Solids]; and
- $NM$  = the number of media in cell.

Note that, by definition, for all species the partition coefficient between the Reference Fluid and itself is 1 (i.e., in the above equation, if  $x$  is the Reference Fluid,  $K_{xi} = 1$ ).

**Read more:** [Creating and Editing Environmental Media](#) (page 64).



**Note:** If the partition coefficients are defined as being independent of the concentration of the species (at a given temperature), the concentrations then vary linearly with mass in the cell (assuming no solubility constraints). This relationship is referred to as a *linear isotherm*. *Non-linear isotherms*, in which the degree of partitioning varies with concentration, can be readily represented in GoldSim by defining the partition coefficients as functions of the concentrations.

**Read more:** [Non-Linear Partitioning](#) (page 297).

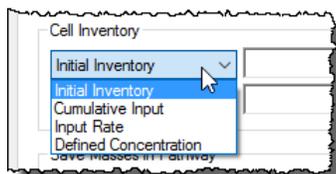
## Defining Initial and/or Boundary Conditions for a Cell

There are four ways by which species mass can enter a Cell:

1. By defining an initial condition and/or a boundary condition for the Cell;
2. By defining discrete changes to the inventory in a Cell;
3. Through a mass flux link from another pathway to the Cell; and/or
4. By associating the Cell with a Source.

Below we discuss the first item, defining an initial and/or boundary condition for a Cell.

An initial condition/boundary condition for a Cell is specified within the “Cell Inventory” section of the dialog. The first field in this section provides four options:



- **Initial Inventory.** This is the default, and represents the initial inventory of each species. This field only accepts vectors by species with dimensions of mass. Moreover, this input cannot be specified as a function of time (if it is, GoldSim will display a fatal error when you try to run the model).
- **Cumulative Input.** This option provides a mechanism for simultaneously specifying an initial condition and a rate of mass addition (that may change with time). This field only accepts vectors by species with dimensions of mass. It represents the *cumulative* amount of mass of each species added to the Cell at a given time. Hence, if it is constant, it represents an initial condition. If it increases with time, its rate of change represents a specified rate of addition. Correct use of the “Cumulative Input” is summarized in the table below:

To specify this:	Enter the following into the "Cumulative Input" field:
An initial condition	A constant vector with dimensions of mass (in this case, however, it would be more transparent to use the "Initial Inventory" option).
An initial condition and a <i>constant</i> rate of addition	An expression such as: $Initial + Rate * Etime$ , where Initial is a constant vector (with dimensions of mass) and Rate is a constant vector (with dimensions of mass/time).
An initial condition and a <i>time-variable</i> rate of addition	The output of a Pool, Reservoir or Integrator element (with output dimensions of mass) with a specified Initial Value and (time-variable) Rate of Change.



**Warning:** The Cumulative Input must stay constant or increase with elapsed time. That is, you cannot remove mass from a Cell using the Cumulative Input field. If the value ever begins to decrease with time, a fatal error occurs.

- **Input Rate.** The third Cell Inventory option is used to specify a rate of mass addition (that may change with time). This field only accepts vectors by species with dimensions of mass/time. It represents the rate at which mass of each species is added to the Cell over the next timestep.
- **Defined Concentration.** The fourth Cell Inventory option is used to specify a concentration boundary condition. This field only accepts vectors by species with dimensions of mass/volume. This option fixes the concentration of each species *in the first fluid listed in the Media list* at the defined level. The concentration represents the dissolved concentration. (If the Cell contains suspended solids, the total concentration could be higher.) The Defined Concentration can be specified as a function of time.



**Note:** One way to easily enter a vector of data into an input field without having to create a separate element is to use GoldSim's vector constructor function. For example, entering "vector(1g)" into the Cumulative Input field results in an initial condition of 1 g of each species being present in the Cell.



**Note:** A **Defined Concentration** boundary condition does not use the specified volume of the first fluid to compute a concentration (it simply applies a specified concentration). However, you should still specify a volume (e.g., 1 m<sup>3</sup>). If you specify a zero volume, it will generate a warning message when you run the model.



**Warning:** A **Defined Concentration** boundary condition can act as both a source and a sink. As a simple example, specifying a concentration of zero would turn the Cell into a sink for mass. Not only would diffusive gradients be toward the Cell, but any mass entering the Cell (by any mechanism) would be removed from the system (in order to maintain a zero concentration).

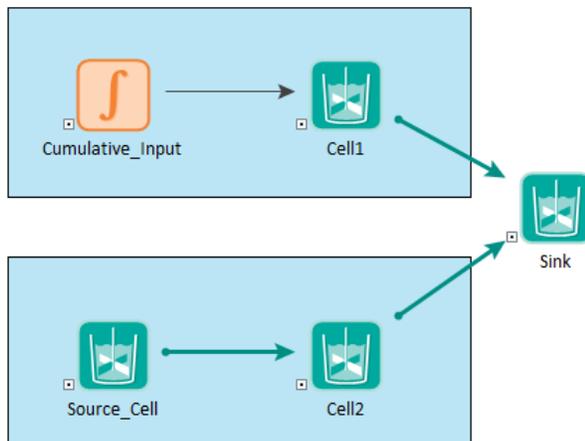


**Warning:** Solubility limits are not applied in Cells with a **Defined Concentration**. If the **Defined Concentration** for a species is above the solubility limit, the solubility limit is ignored, the **Defined Concentration** is applied, and a warning is written to the Run Log.

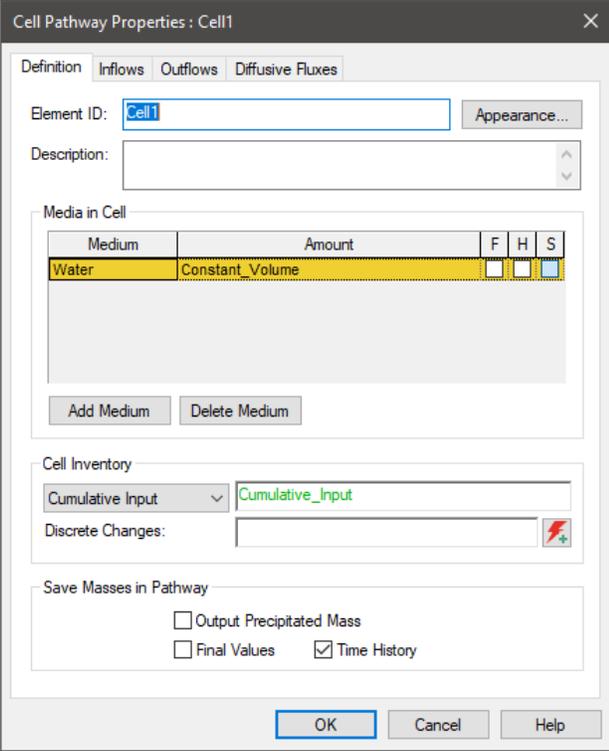
**Read more:** [Simulating Solubility Limits in Cells](#) (page 159).

Although the **Input Rate** and **Cumulative Input** options provide a quick and convenient way to enter mass input rates, if mass input rates into a Cell are changing with time (e.g., because the inflow concentration is changing), a slightly more accurate way (both numerically and conceptually) to specify such a boundary condition is to create a second Cell that is defined using a **Defined Concentration**.

As an example, consider a case in which you have a boundary condition with a constant inflow rate (Flow\_Rate) and a time-varying Inflow\_Concentration. There is also an Initial\_Concentration in the Cell, which has a Constant\_Volume and constant outflow rate (equal to the inflow rate). You could model this in two ways, as illustrated in the example below:



The example in the top uses the **Cumulative Input** option for the “Cell Inventory” in Cell1:



Cell Pathway Properties : Cell1

Definition Inflows Outflows Diffusive Fluxes

Element ID:  Appearance...

Description:

Media in Cell

Medium	Amount	F	H	S
Water	Constant_Volume	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Add Medium Delete Medium

Cell Inventory

Cumulative Input

Discrete Changes:

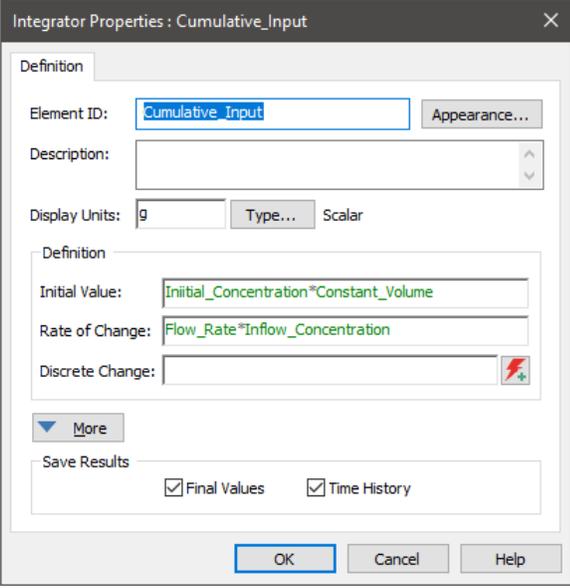
Save Masses in Pathway

Output Precipitated Mass

Final Values  Time History

OK Cancel Help

The Cumulative\_Input Integrator element is defined as follows (with an initial mass and a mass input rate):



Integrator Properties : Cumulative\_Input

Definition

Element ID:  Appearance...

Description:

Display Units:  Type... Scalar

Definition

Initial Value:

Rate of Change:

Discrete Change:

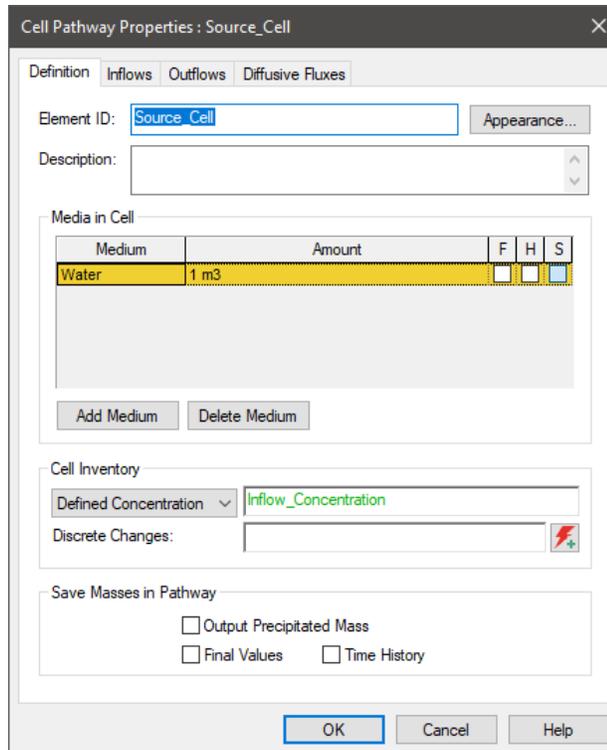
More

Save Results

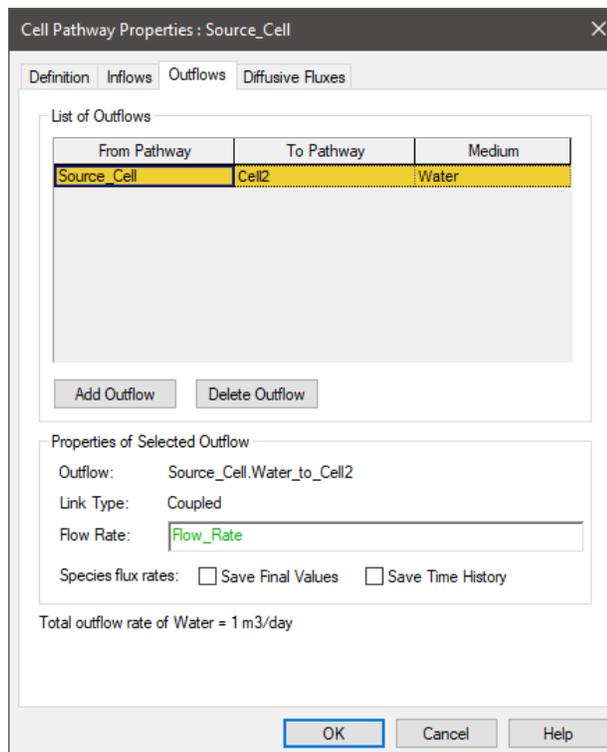
Final Values  Time History

OK Cancel Help

The example on the bottom defines a “Source\_Cell” that looks like this:



The volume is set to an arbitrarily small number (it is not used to compute concentrations since the concentration is fixed). A **Defined Concentration** is specified for this Source\_Cell that will flow into Cell2. That is, the Source\_Cell has an outflow to Cell2:



Cell2 looks like this:

Cell Pathway Properties : Cell2

Definition Inflows Outflows Diffusive Fluxes

Element ID:  Appearance...

Description:

Media in Cell

Medium	Amount	F	H	S
Water	Constant_Volume	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Add Medium Delete Medium

Cell Inventory

Initial Inventory

Discrete Changes:

Save Masses in Pathway

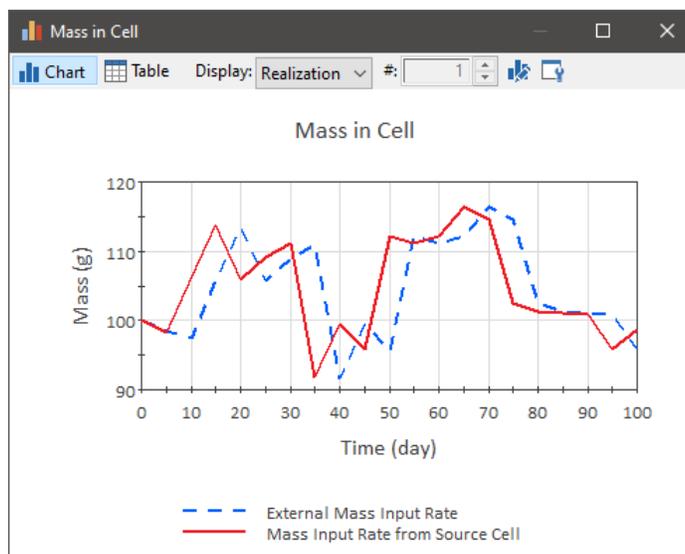
Output Precipitated Mass

Final Values  Time History

OK Cancel Help

It has an **Initial Inventory**, as well as an inflow from the Source\_Cell.

If we run this model (for 100 days with a 5 day timestep) and compare the results for these two different approaches to representing the boundary condition (in terms of mass in Cell1 and Cell2), they look like this:



What we see is that the mass that is input “externally” (using the **Cumulative Input**) lags by one timestep. This is because in this approach (or in the absence of an initial condition, using an **Input Rate**), due to the way the external boundary condition must be applied when solving the pathway equations, a one timestep lag is introduced. Hence, the second approach is a more accurate representation (although for a small timestep, the differences would likely be insignificant). Conceptually, however, this is a bit more accurate way to

## Simulating Discrete Changes to the Mass Inventory in a Cell

represent the boundary condition (since the boundary condition is actually treated as part of the pathway network).

In addition to adding mass to a Cell via an initial/boundary condition, and adding/removing mass via mass flux links, GoldSim allows you to instantaneously add, remove or redefine (replace) the amount of species mass in a Cell.

This is done using the Discrete Changes field in the Cell dialog, which is located within the “Cell Inventory” section:

The screenshot shows a dialog box titled "Cell Inventory". It contains two input fields. The first is a dropdown menu labeled "Initial Inventory" with a downward arrow. The second is a text input field labeled "Discrete Changes:" with a red lightning bolt icon to its right.

This field only accepts discrete change signals. (Discrete change signals are discussed in detail in "Simulating Discrete Events" in the **GoldSim User's Guide**.) The discrete change signal must be a vector by species and have dimensions of mass. Typically, such a discrete change signal will be the output of a Discrete Change element that has been triggered by an event.

Discrete change signals have an *instruction* associated with them. Two types of instructions are possible: Add and Replace. The Discrete Changes field for a Cell accepts both Add and Replace signals.

When an Add signal is sent to a Cell during a simulation, the specified amount of mass of each species in the discrete change vector is added to the current mass in the pathway. If the vector contains negative values, mass is subtracted from the pathway for those species which have negative values.



**Note:** The mass is added (or subtracted) uniformly over a timestep previous to when the discrete change occurred. For example, if you had a 10-day timestep, and an event occurred (which interrupted the clock) which added mass at 35 days, the mass would be added uniformly between 30 and 35 days.



**Note:** Because a pathway cannot contain a negative amount of species mass, GoldSim will not remove more mass from the pathway than is present. That is, if the discrete change signal specifies that a quantity of species mass is to be subtracted which exceeds the current species mass in the pathway, GoldSim will stop the simulation and display a fatal error message.

When a signal with a Replace instruction is sent to a Cell during a simulation, the specified amount of mass completely replaces the current mass values in the pathway.



**Note:** Because a pathway cannot contain a negative amount of species mass, GoldSim will not replace the current mass with a negative value. That is, if the Replace signal specifies a negative quantity of species mass, GoldSim will stop the simulation and display a fatal error message.

Like most input fields that accept discrete change signals, you can specify multiple discrete changes. You can do this in two ways:

1. You can enter multiple discrete changes into the input field by separating the entries using a semi-colon; and
2. You can use the Multiple Discrete Changes button to the right of the input field (i.e., the small button with two exclamation marks) to access a table listing the Discrete Changes (to which you can add or delete entries).

In the latter case, any Discrete Changes which are added to the list are also automatically added to the input field, separated by semi-colons.

The Discrete Changes field can be very useful for instantaneously modifying your system in response to discrete events. Note, however, that this feature should be used with care, since when it is applied, conservation of mass in the system is the responsibility of the user.

## Cell Pathway Outputs

Cell pathways have at least one output:

- **Mass\_in\_Pathway.** This is a vector by species with dimensions of mass. It represents the total mass of each species in the Cell.



**Note:** The Mass\_in\_Pathway output is the primary output for the Cell. Hence, if you right click on a Cell in Result Mode and select a result to display, it will display the Mass\_in\_Pathway output.

In addition, if the **Output Precipitated Mass** checkbox is selected at the bottom of the Cell dialog, an additional output is added to the Cell:

- **Precipitated\_Mass.** This is a vector by species with dimensions of mass. It represents the total amount of mass of each species in the Cell that is currently precipitated.



**Note:** Precipitated\_Mass can be non-zero even in the absence of solubility limits. If none of the Fluids in the Cell have non-zero volumes, then any mass in the Cell will precipitate out onto any Solids present in the Cell (proportional to the mass of each Solid) even if no solubility limit is specified.

For every medium that you add to the Cell, an output is created on the Cell:

- **Concentration\_in\_Medium,** where *Medium* is the name of the medium you have added. This is a vector by species. If the medium is a fluid, it has dimensions of mass per volume. If the medium is a solid, it has dimensions of mass per mass.

If one or more Solids are suspended in a Fluid, the fluid concentration is computed as the *effective* concentration, which includes the suspended solids:

$$c_i = cd_i + \sum_{k=1}^{NK} \frac{m_{\text{part},k}}{V} csorb_{k,i}$$

where:

- $c_i$  is the effective concentration in the fluid (M/L<sup>3</sup>);
- $cd_i$  is the dissolved concentration in the fluid (M/L<sup>3</sup>);

$m_{\text{part},k}$	is the mass of particulate solid $k$ in the cell (M);
$V$	is the volume of the fluid in cell ( $L^3$ );
$csorb_{k,i}$	is the concentration of species $i$ in particulate solid $k$ (M/M); and
$NK$	is the number of solids suspended in the fluid.

If the Cell contains a suspended Solid, then an additional output is added:

- **Dissolved\_Conc\_in\_Fluid**, where *Fluid* is the name of the fluid directly above the suspended Solid in the list or media. It represents the dissolved concentration of species in the fluid (excluding the contribution from suspended solids). This is a vector by species. It has dimensions of mass per volume.

Finally, GoldSim also creates a Cell output for each mass flux link created from the Cell to other pathways. Two types of mass flux links can be created from a Cell: advective links and diffusive links.

**Read more:** [Creating Mass Flux Links](#) (page 90).

For every advective mass flux link in which the Cell is the Outflow (upstream) pathway, an output is created on the Cell:

- **Medium\_to\_Path2**, where *Medium* is the name of the flowing medium, and *Path2* is the name of the linked (Inflow) pathway. This is a vector by species, and has dimensions of mass/time. It represents the mass flux of each species from the Cell to the downstream pathway.

**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94).

For every diffusive mass flux link in which the Cell is the Outflux pathway, an output is created on the Cell:

- **Medium1\_to\_Medium2\_in\_Path2**, where *Medium1* is the name of the fluid on the Outflux side of the link, *Medium2* is the name of the fluid on the Influx side of the link, and *Path2* is the name of the linked (Influx) pathway.

**Read more:** [Inputs and Outputs Associated with Diffusive Mass Flux Links](#) (page 101).

For every direct transfer mass flux link in which the Cell is the Outflow (upstream) pathway, an output is created on the Cell:

- **Direct\_transfer\_rate\_to\_Path2**, where *Path2* is the name of the linked (Inflow) pathway. This is a vector by species, and has dimensions of mass/time. It represents the mass flux of each species from the Cell to the downstream pathway.

**Read more:** [Inputs and Outputs Associated with Direct Transfer Mass Flux Links](#) (page 105).

For every precipitate removal mass flux link in which the Cell is the Outflow (upstream) pathway, an output is created on the Cell:

- **Precipitate\_transfer\_rate\_to\_Path2**, where *Path2* is the name of the linked (Inflow) pathway. This is a vector by species, and has dimensions of mass/time. It represents the mass flux of each species from the Cell to the downstream pathway.

**Read more:** [Inputs and Outputs Associated with Precipitate Removal Mass Flux Links](#) (page 110).

For every treatment mass flux link in which the Cell is the Outflow (upstream) pathway, an output is created on the Cell:

- **Fraction\_of\_inflows\_to\_Path2**, where *Path2* is the name of the linked (Inflow) pathway. This is a vector by species, and has dimensions of mass/time. It represents the mass flux of each species from the Cell to the downstream pathway.

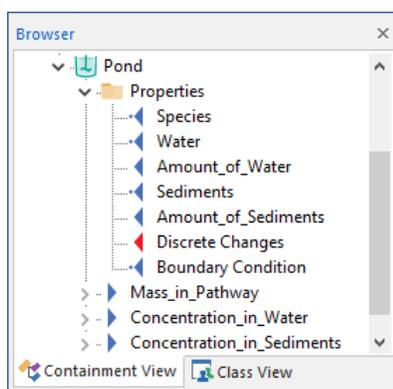
**Read more:** [Inputs and Outputs Associated with Treatment Mass Flux Links](#) (page 116).

It is important to understand that the mass flux outputs from a Cell represent the mass rate over the *previous* timestep. This can have implications if you choose to integrate one of these outputs (using an Integrator).

**Read more:** [Manipulating Pathway Outputs](#) (page 253)

## Viewing a Cell in the Browser

The browser view of a Cell pathway is shown below:



The *Properties* folder contains the basic inputs for the Cell, including the Boundary Conditions, Discrete Changes, and the quantities of the media present.



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

The pathway's mass and concentration outputs are listed first. Note that in this particular example, the Cell contains two media: Water (the Reference Fluid), and Sediments.

The Properties folder contains the basic inputs for the Cell. In particular, it contains the Cumulative Input, Discrete Changes, and the quantities of each of the media present. You can create links to these inputs using the Link Cursor.

Note that the Species input, and an input for each medium in the cell also appear in the Properties folder. The Species input is automatically linked to the nearest Species element when the Cell is created. The media inputs are automatically created and linked to the corresponding media when they are added to the cell. *These links cannot be changed using the Link Cursor, and are displayed for information purposes only.*

If the Cell has any mass flux links associated with it, the corresponding inputs and outputs for these links are organized into the Inflows, Outflows, Diffusive

Influxes, and Diffusive Outfluxes folders. Note that these folders are not shown if they are empty.

**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94); [Inputs and Outputs Associated with Diffusive Mass Flux Links](#) (page 101); [Inputs and Outputs Associated with Direct Transfer Mass Flux Links](#) (page 105); [Inputs and Outputs Associated with Precipitate Removal Mass Flux Links](#) (page 110); [Inputs and Outputs Associated with Treatment Mass Flux Links](#) (page 116).

## Advective Flux Links to/from Cells

Perhaps the simplest way to transport mass out of or into a Cell is by specifying an advective mass flux link to or from another pathway.

**Read more:** [Understanding Advective Mass Flux Links](#) (page 90).

Advective mass flux links are used to transport mass via a flowing medium. Mass which is dissolved in, or sorbed onto suspended in the flowing medium is transported with the medium as it moves. Hence, an advective mass flux is computed as the concentration of the mass in the medium multiplied by the rate at which the medium is flowing:

$$\text{Advective Mass Flux} = \text{Concentration} * \text{Flow Rate}$$

For Cell pathways, the flowing medium can be a Fluid or a Solid.

It is important to understand that the quantity of a medium in a Cell is specified directly by the value in the media list for the Cell. These values are not changed by the specified Outflows and/or Inflows of that medium from/to the Cell. That is, even though you specify the rate at which the medium leaves (and/or enters) the Cell when you create an advective flux, this has no effect on the quantity of the medium in the Cell(s). GoldSim uses the advective rates only to transport mass and does not keep track of the movement of media (e.g., Water) through the pathway network.

**Read more:** [Understanding How Cells Manage Flow Balance](#) (page 164).

## Cell Pathway Example #2: Advective Flux Links

It is worthwhile to examine a simple example of an advective flux link between Cells. This particular example file, Cell2\_Advection.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

Suppose that 10 g of chemical A and B is released into a small pond. The pond contains two media: Water and Sediments. Neither species decays. A sorbs onto the Sediments. This sorption can be quantified by specifying a partition coefficients for A (equal to 4 m<sup>3</sup>/kg). B does not sorb. Because the pond is shallow, it is assumed that it is well-mixed, and the Water and Sediments are instantaneously at equilibrium with respect to partitioning of the species.

Finally, assume that Water is pumped from the pond at a rate of 50 m<sup>3</sup>/yr. We assume that none of the Sediments leave the pond with the Water. Moreover, clean Water is pumped into the pond at the same rate (so the pond volume stays constant).

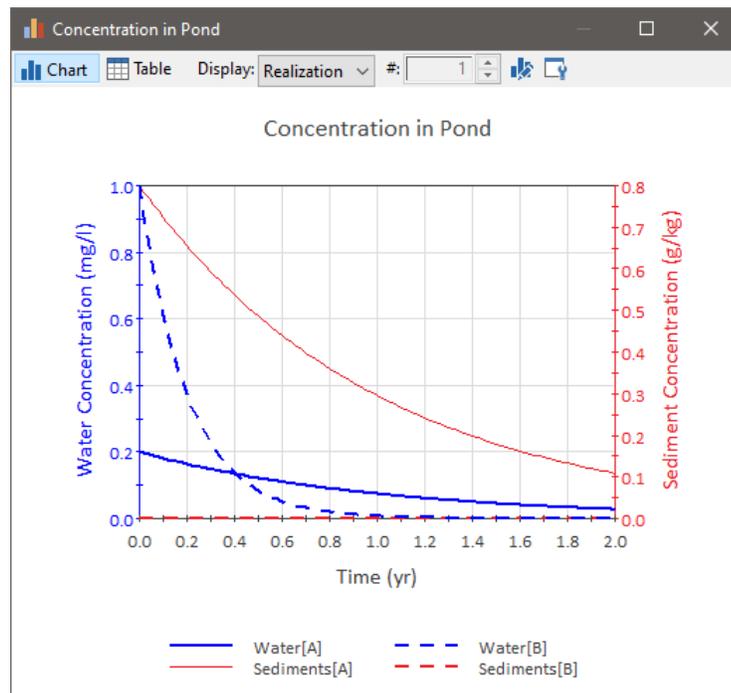
You wish to predict the concentration of the two species in the Water and Sediments in the pond as a function of time.

To simulate this system in GoldSim, you would do the following:

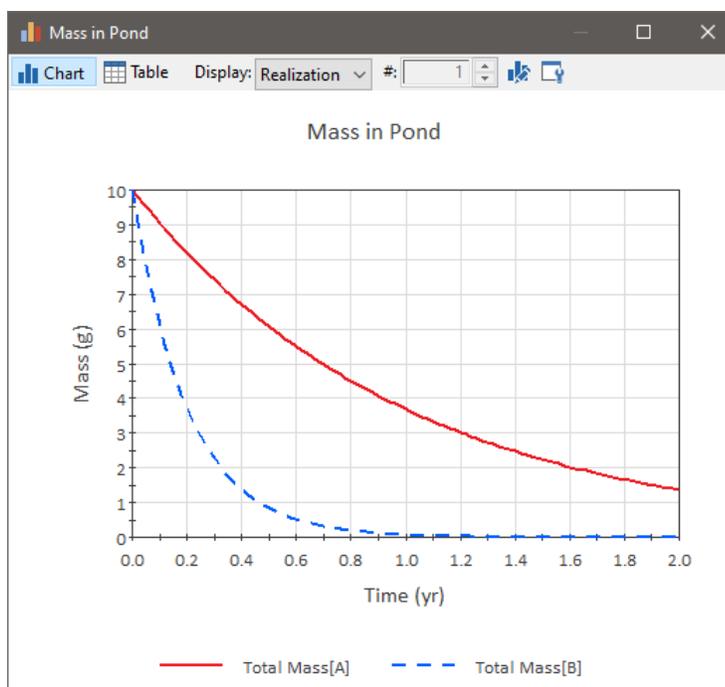
1. Define two species (A and B);
2. Define two media (Water and Sediments) and specify their properties;
3. Define a Cell pathway to represent the pond;

4. Define a second Cell pathway to represent the location to which the pond discharges;
5. Specify the quantities of Water and Sediment present in the pond Cell (the amount in the downstream Cell is unimportant as this just represents a sink);
6. Specify an initial mass of species in the pond Cell;
7. Create an advective flux link from the Pond to the downstream Cell and specify the quantity of Water flowing; and
8. Specify the simulation settings (i.e., duration and timesteps), and run the model.

The output of this simulation, in the form of time histories of the concentrations of species A and B in the Water and Sediments in the Pond, is shown below:



Note that B decreases at a much faster rate than A. This is because B is not sorbed onto the Sediments at all (the concentration of B in Sediments is 0). Hence, it flushes from the system much faster. Because A is sorbed onto the Sediments (and only Water is flushed from the pond, not the Sediments), it takes much longer to leave the system. This is made more apparent by looking at the total mass of each species in the Cell (as opposed to the concentrations in Water and Sediments):



### Advection of Particulates to/from Cells

If one or more Solids are suspended in a Fluid, the fluid concentration that is output is computed as the *effective* concentration, which includes the species mass associated with the suspended Solids.

Note that when a suspended Solid is present in a Cell, an additional output is created called *Dissolved\_Conc\_in\_Fluid*, where *Fluid* is the Fluid in which the Solid is dissolved (typically water). This output provides the actual concentration of dissolved species in the Fluid. The *Concentration\_in\_Fluid* output provides the *effective* concentration of species in the Fluid (accounting for species sorbed onto suspended solids).

**Read more:** [Cell Pathway Outputs](#) (page 133); [Defining Suspended Solids in a Cell](#) (page 124).

Advective mass flux links involving Fluids containing suspended Solids transport both the species mass dissolved in the fluid *and* the species mass associated with (partitioned onto) the suspended Solid(s).

With regard to the transport of species mass on particulates from Cells, the following rules are followed:

- If the advective mass flux link is between two Cells, then the particulates are only advected into the downstream (Inflow) Cell if the Solid exists in that Cell. (The Solid does not have to be specified as being suspended in the Inflow Cell, but it must exist in that Cell.) If it does not, GoldSim assumes that the Solid particulates are "filtered" out before entering the Inflow Cell (and remain in the Outflow Cell).
- If the advective mass flux link is between a Cell and any other type of pathway, the particulates are always transported with the flowing fluid.
- If the Solid is not suspended in the Inflow Cell (or the Inflow pathway is not a Cell), conceptually, the particulates are assumed to immediately disintegrate upon entering the Inflow pathway, with the species mass which was associated with them instantaneously partitioning among the available media in the pathway.

- The Solid's Advective Velocity Multiplier (an Advanced property of the Solid medium) can increase the mass flux associated with the suspended Solid. The Advective Velocity Multiplier effectively controls the velocity (and hence the mass flux) of the advected particulate Solid relative to the advecting Fluid. The default value is 1 (it moves at the same velocity as the Fluid). But you can choose to have the suspended Solid move faster or slower than the Fluid.

**Read more:** [Advanced Solid Properties](#) (page 77).

- For computational reasons, the mass in a Cell in excess of the saturation capacity (the "precipitated" mass) is assumed to be precipitated only onto those Solids which are not suspended. Hence, although species mass can be partitioned onto (and transported with) particulate Solids, *precipitated* species mass is never associated with suspended Solids.

**Read more:** [Simulating Solubility Limits in Cells](#) (page 159).

As is the case for the advecting Fluid itself, GoldSim uses the advective flux only to transport species mass and does not keep track of the movement of the suspended Solid media through the pathway network. That is, the advective flux has no effect on the quantity of the suspended Solid present in either the Outflow or Inflow Cell.

## Diffusive Flux Links to/from Cells

In addition to transporting mass out of or into Cells via advective mass flux links, mass can also be transported via diffusive mass flux links.

**Read more:** [Understanding Diffusive Mass Flux Links](#) (page 95).

Diffusive mass flux links are used to transport mass through a fluid via the process of molecular diffusion. Diffusive mass transport is driven by a concentration gradient, with mass diffusing from high concentration to low concentration. The constant of proportionality is referred to as the *diffusive conductance*:

$$\text{Diffusive Mass Flux} = (\text{Diffusive Conductance}) * (\text{Concentration Difference})$$

The diffusive conductance is a function of the properties of the species and fluids involved, and the geometry of the diffusive process. This is discussed in detail in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

Diffusive mass flux links between Cells are bi-directional (mass can be transported in either direction). The pathway from which the link was created is referred to as the Outflux pathway, and the other pathway in the link is referred to as the Influx pathway. Diffusive fluxes away from the Outflux pathway are, by convention, positive.



**Note:** If the volume of the Fluid associated with a diffusive flux link goes to zero, a fatal error will occur. That is, you cannot simulate diffusion through a system in which the volume of the fluid through which the mass is diffusing goes to zero.

---

## Specifying the Geometry of Diffusive Flux Links

A diffusive flux link between two pathways has two "sides".

**Read more:** [Understanding Diffusive Mass Flux Links](#) (page 95).

The geometry of the flux link is defined by three inputs:

- the diffusive length on the Outflux side of the link;
- the diffusive length on the Influx side of the link; and
- the diffusive area of the link.

In effect, the Cells act as "nodes" and a collection of Cells linked by diffusive mass fluxes is mathematically identical to a finite difference approximation of the system.

A single diffusive mass flux link between two pathways mathematically represents a *one-dimensional* diffusive process. For example, if you wished to simulate diffusion along a one-dimensional conduit, you would do so as follows:

1. Specify how you wished to discretize the system by defining the number of Cells you use to represent the conduit.
2. Create diffusive mass flux links between adjacent Cells. The diffusive area would be the same for all mass flux links, and would be equal to the cross-sectional area of the conduit. The diffusive length for each side of each diffusive mass flux link would be equal to half the effective "length" of each Cell. Hence, if you were simulating a 10 m conduit using 5 Cells, each Cell would have an effective length of 2 m, and the diffusive length on each side of each diffusive mass flux link would be specified as 1m.

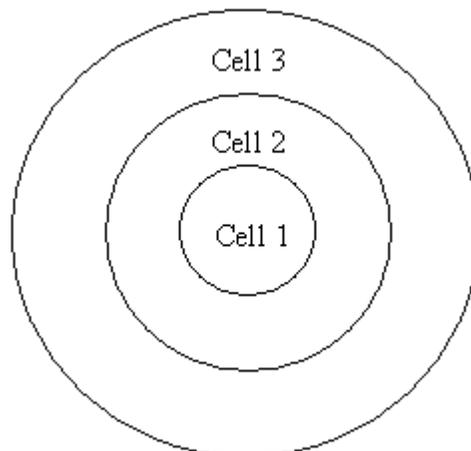


**Note:** The amount of media in each Cell (i.e., the size of the Cell) should be defined in a manner that is consistent with the diffusive lengths and areas. For example, in a one-dimensional system simulated using equal sized Cells (filled only with water), the volume of water in each Cell would be equivalent to twice the diffusive length multiplied by the diffusive area.

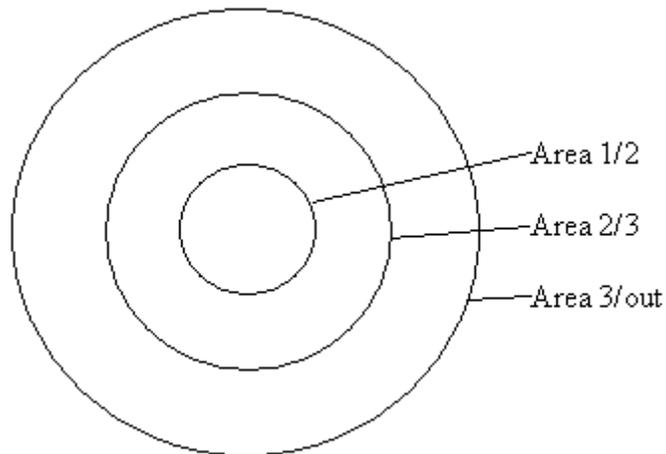
---

By linking multiple Cells together via diffusive mass flux links and defining the size (volume) of the Cells and the diffusive lengths and areas appropriately, nearly any geometry can be numerically represented by such a network of cells. For example, to represent the diffusion from the center of a sphere outward, you would do the following:

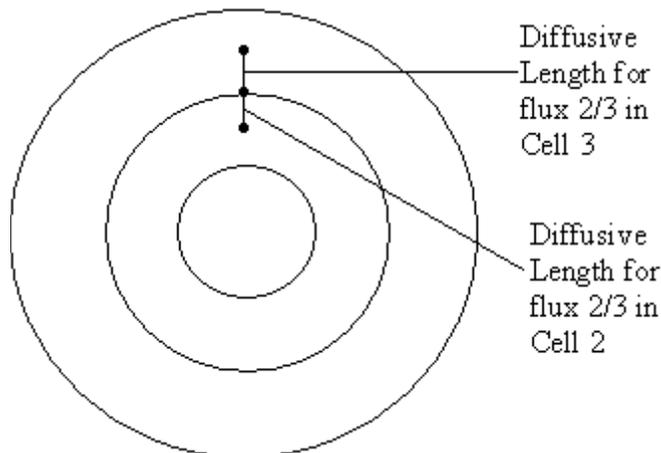
1. Divide the sphere into a number of "shells", with the volume between the shells defining each Cell:



2. Create diffusive mass flux links between adjacent Cells. For each link, the diffusive area would be computed as the surface area of the shell separating the two Cells:



Similarly, the diffusive length for each side of each diffusive mass flux link would be computed as the distance from the “midpoint” of the Cell to the shell shared by the two Cells:



### ***Diffusion of Particulates to/from Cells***

If one or more Solids are suspended in a Fluid, the Solid particulate matter itself can diffuse, driven by the concentration gradient of the Solid. Any species mass associated with (partitioned onto) the suspended Solid(s) will be transported with the diffusing Solid.

**Read more:** [Defining Suspended Solids in a Cell](#) (page 124).

With regard to the transport of species mass on particulates from Cells, the following rules are followed:

- If the diffusive mass flux link is between two Cells, then the particulates are only diffused into the Influx Cell if the Solid (or a Solid with the same name) exists in that Cell. (The Solid does not have to be specified as being suspended in the Influx Cell, but it must exist in that Cell.) If it does not, GoldSim assumes that the Solid particulates are “filtered” out before entering the Influx Cell (and remain in the Outflux Cell).
- If the diffusive mass flux link is between a Cell and any other type of pathway, the particulates always diffuse into the Influx pathway.

- For computational reasons, the mass in a Cell in excess of the saturation capacity (the "precipitated" mass) is assumed to be precipitated only onto those Solids which are not suspended. Hence, although species mass can be partitioned onto (and transported with) particulate Solids, *precipitated* species mass is never associated with suspended Solids.

**Read more:** [Simulating Solubility Limits in Cells](#) (page 159).

If the Solid is not suspended in the Influx Cell (or the Influx pathway is not a Cell), the suspended Solid concentration in that pathway is simply assumed to be zero when computing the diffusive gradient (and, hence, the diffusive flux becomes uni-directional). Conceptually, the particulates are assumed to immediately disintegrate upon entering the Influx pathway, with the species mass which was associated with them instantaneously partitioning among the available media in the pathway.

The diffusivity of particulate Solids is specified when defining the properties of the Solid.

**Read more:** [Advanced Solid Properties](#) (page 77).

As is the case for the advecting Fluids and particulates, GoldSim uses the diffusive flux of particulates only to transport species mass and does not keep track of the movement of the suspended Solid media through the pathway network. That is, the diffusive flux of particulates has no effect on the quantity of the suspended Solid present in either the Outflux or Influx pathway.

When diffusion is taking place through a fluid (typically water or air) that only partially saturates the porous medium, this can reduce the diffusive flux. You can account for this by defining a Diffusivity Reduction Formula for each Fluid in your model.

Within GoldSim, the diffusive mass transport is computed as follows:

$$\text{Diffusive Mass Rate} = (\text{Diffusive Conductance}) * (\text{Concentration Difference})$$

In this equation, the Diffusive Mass Rate has dimensions of mass/time, the Diffusive Conductance has dimensions of volume/time, and the Concentration Difference has dimensions of mass/volume.

Assuming that the species are diffusing through a single fluid, the Diffusive Conductance term is computed as follows:

$$D = (A d t n r) / L$$

where:

D is the Diffusive Conductance ( $L^3/T$ );  
 A is the diffusive area ( $L^2$ );  
 d is the diffusivity in the fluid ( $L^2/T$ );  
 n is the porosity of the porous medium;  
 t is the tortuosity of the porous medium;  
 r is the Diffusivity Reduction (the default value is 1); and  
 L is the diffusive length (L).

d and r are Fluid properties, and t and n are Solid properties.

**Read more:** [Fluid Properties](#) (page 69); [Basic Solid Properties](#) (page 75).

### **Diffusion Through Partially Saturated Porous Media**



**Note:** If the diffusion is not taking place through a porous medium,  $t$ ,  $n$  and  $r$  in this equation are all effectively set to 1.

The Diffusivity Reduction Formula is a Fluid property (i.e., it is defined in the Reference Fluid or Fluid property dialog). The Diffusivity Reduction Formula is a dimensionless value that has the impact of decreasing the effective diffusivity based on the the fluid's saturation level within any Cell pathways in which it is present.

When used, this formula is intended to directly reference the fluid's saturation level using a special local available property called "Saturation". It must be referenced as "~Saturation" in the equation entered into the field:

Note that the ~Saturation local available property can only be referenced directly in this field; it cannot be used in a separate element that is then linked into this field.



**Note:** Locally available properties are discussed in detail in Chapter 10 of the **GoldSim User's Guide**.

When the fluid is used within a Cell pathway, GoldSim internally computes the saturation of the fluid in the pathway, and uses this value to compute the Diffusivity Reduction Formula (and hence the diffusive mass flux) into and out of the Cell. For each Cell, the saturation level of each fluid is computed by GoldSim as follows:

1. The combined pore volume of all (non-suspended) Solid media is computed as:

$$\text{Combined Pore Volume} = \Sigma (\text{Mass of Solid} * \text{Porosity} / \text{Bulk Density})$$

where the summation is over all solids.

2. For the first Fluid in the Cell, the Saturation is computed as:

$$\text{Saturation} = \min(\text{Fluid Volume}, \text{Combined Pore Volume}) / \text{Combined Pore Volume}$$

3. If there are additional fluids in the Cell, the Saturation for each Fluid is computed, in turn, as:

$$\text{Saturation} = \min(\text{Fluid Volume}, \text{Remaining Unfilled Pore Volume}) / \text{Combined Pore Volume}$$

This method of computing saturation has two important implications:

- The first Fluid listed in the Cell is treated as the wetting fluid (it is the first fluid to fill the pores).
- If the Cell contains multiple Solids, the fluids have access to the pore space in all the Solids simultaneously (i.e., the pore space of Solids are not filled in a specific order).

Conceptually, the Diffusivity Reduction Formula should equal 1 when the saturation is equal to 1 (and 0 when the saturation is equal to 0). As a result, one convenient form for the Diffusivity Reduction Formula is:

$$\text{Diffusivity Reduction Formula} = \sim\text{Saturation}^E$$



**Note:** The impact of saturation on the diffusion rate is complex. While the Diffusivity Reduction Formula (when defined appropriately as a function of saturation) reduces the effective diffusivity, a lower saturation changes the volume of water available. This in turn affects the concentration (and hence the concentration gradient). Moreover, decreasing the volume of water available increases the retardation due to sorption (since all of the mass of the porous medium is still assumed to be available, but only a fraction of the water is).

---

### **Inter-media Diffusion**

A diffusive mass flux link between two pathways has two "sides" (one for each of the linked pathways). Mass diffuses from one pathway, through the "diffusive layer" on one side of the link, through the "diffusive layer" on the other side of the link, and into the other pathway.

**Read more:** [Creating and Editing Diffusive Mass Flux Links](#) (page 98).

Note that the two fluids on either side of the link do not have to be identical. For example, you could connect two cells via a diffusive link with Water on one side of the link and Air on the other. In fact, transfer across the air-water interface (e.g., of a lake) is often mathematically represented in this way.

In such a situation, when a species diffuses through one side of the link, it must partition from one fluid into the other before it can diffuse through the other side of the link. GoldSim handles this partitioning automatically, based on the specified partition coefficient(s) for the species to the two fluids.



**Warning:** Particulate Solids will not diffuse in a link in which the two fluids on either side of the link do not have the same name (since typically it would be inappropriate to assume that a particulate solid would "partition" between fluids.) If you wish to transport Solids across a fluid interface, you can do so by defining an advective mass flux link between the pathways involving the Solid.

---

### **Cell Pathway Example #3: Diffusive Flux Links**

To illustrate the use of diffusive flux links, we consider a simple case involving intermedia diffusion across an air/water interface. This particular example file, Cell3\_Diffusion.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

Suppose that a closed beaker contains 1 liter of water and 1 liter of air. The air-water interface has an area of 20 cm<sup>2</sup>. 1 mg of a volatile organic compound is injected into the water, with a Henry's Law constant (the partition coefficient between air and water) equal to 10 m<sup>3</sup>/m<sup>3</sup>. The water and air in the beaker are gently stirred, so that you can assume that the water and air portions are well-

mixed. You wish to simulate the transfer of the compound across the air-water interface. In particular, you want to know how long it takes for the system to reach equilibrium.

Such a transfer process is often modeled by assuming that the interface can be represented by two boundary layers: one on the water side, and one on the air side. Because both the air and water are assumed to be well-mixed, the concentration within the bulk of the air and water (outside of the boundary layers) is assumed to be uniform. Therefore, the kinetics of the transfer process are controlled by the diffusion of the organic from the bulk water through the water boundary layer, the (instantaneous) partitioning from water to air at the interface, and the diffusion for the organic through the air boundary layer into the bulk air. For the purposes of this example, we assume that the water boundary layer has a thickness of 0.1 mm, and the air boundary layer has a thickness of 5 mm.



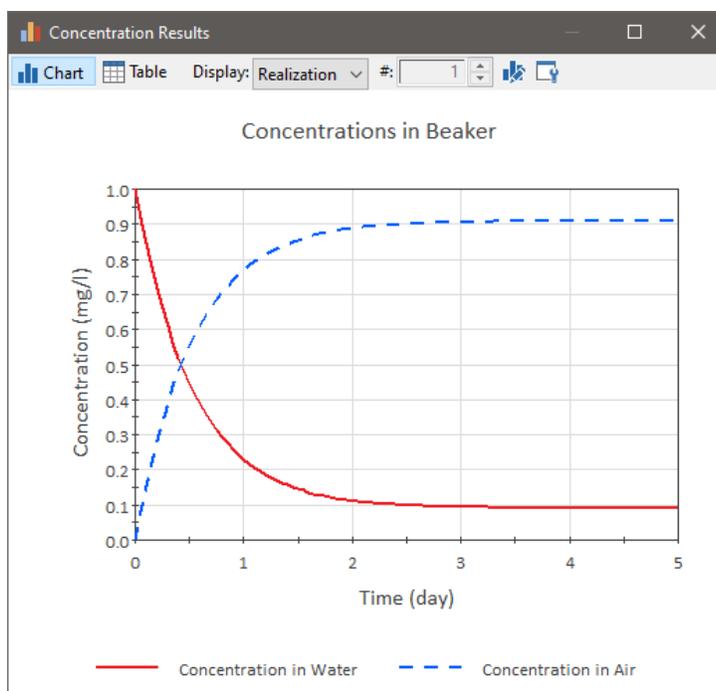
**Note:** Due to the nature of turbulence, air boundary layer thickness are (perhaps somewhat counter-intuitively) significantly larger than water boundary layer thicknesses. Note, however, that due to the fact that the diffusivity of chemicals in air are on the order of four orders of magnitude greater than in water, unless the Henry's Law constant is relatively small, the water boundary layer controls the process (i.e., the resistance of the air boundary layer is negligible). That is indeed the case in this example, in which the Henry's Law constant is quite large.

---

To simulate this system, you would do the following:

1. Create a fluid called Air and assign it an appropriate reference diffusivity value ( $1E-5$  m<sup>2</sup>/sec) and define the Henry's Law constant;
2. Define a Water\_Side Cell containing 1 liter of Water;
3. Define an Air\_Side Cell containing 1 liter of Air;
4. Create a diffusive flux link between the Water\_Side cell and the Air\_Side cell.
5. Specify the simulation settings (i.e., duration and timesteps), and run the model.

The output of this simulation, in the form of time histories of the concentrations of the organic in both Cells, is shown below:



Note that it takes about two days for the system to reach equilibrium. At equilibrium, the concentration in the Air is ten times higher than the concentration in Water (i.e., exactly equal to the Henry's Law constant).

## Direct Transfer Flux Links to/from Cells

Direct transfer mass flux links are used to transport mass directly from one pathway to another via a mechanism that cannot be appropriately represented as either advection or diffusion. They are defined by specifying a fractional rate at which mass is being moved from one pathway to another. Hence, a direct transfer mass flux is computed as the mass of the species in the pathway multiplied by a fractional transfer rate:

$$\text{Direct Transfer Mass Flux} = \text{Mass in Cell} * \text{Transfer Rate}$$

The Transfer Rate has dimensions of inverse time. The Transfer Rate is specified as a vector by species. This allows the Transfer Rate to be species-specific.

Direct transfer mass flux links are uni-directional (mass can only be transported in one direction). That is, the Transfer Rate must be non-negative.

## Cell Pathway Example #4: Direct Transfer Flux Links

To illustrate the use of direct transfer flux links, consider a simple case involving direct transfer of a species from one Cell (representing soil) to another Cell (representing plant material). This particular example file, Cell4\_DirectTransfer.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

Suppose that a jar contains 1 kg of soil. The soil contains 1 gram each of two species; species A is not taken up by the plant. Species B, however, is absorbed by the plant as a first order process (i.e., at a rate proportional to the amount of mass in the soil cell). The transfer rate is 10% per day.

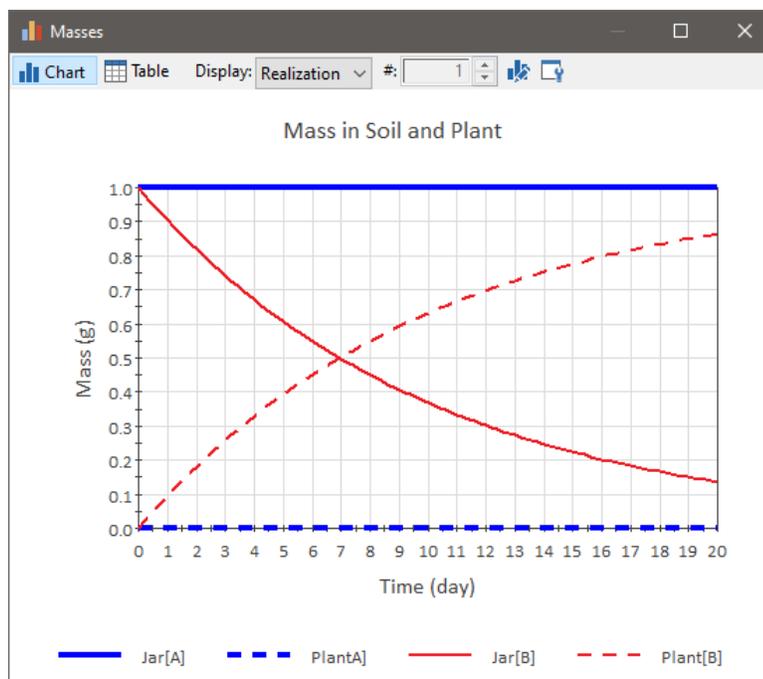
You wish to simulate the transfer of the compound from the soil into the plant.

To simulate this system, you would do the following:

1. Create a solid called Soil and a solid called Plant\_Material;

- Define a Jar Cell containing 1 kg of Soil;
- Define a Plant Cell containing 1 g of Plant\_Material (the amount of Plant\_Material is not important, as the Plant Cell is simply acting as a sink);
- Create a direct transfer flux link between the Jar Cell and the Plant Cell.
- Specify the simulation settings (i.e., duration and timesteps), and run the model.

The output of this simulation, in the form of time histories of the masses of the two species in both Cells, is shown below:



Note that the mass of species A does not change in either Cell, while the mass of species B decreases exponentially in the Jar Cell (and increases accordingly in the Plant Cell).

## Precipitate Removal Flux Links to/from Cells

Precipitate removal mass flux links are used to transport precipitated mass directly from one pathway to another. Mass can precipitate in a Cell if solubility limits have been defined for the species in the fluid within the Cell.

**Read more:** [Simulating Solubility Limits in Cells](#) (page 159).

They are defined by specifying a fractional rate at which the precipitated mass is being moved from one pathway to another. Hence, a precipitate removal mass flux is computed as the precipitated mass of the species in the pathway multiplied by a fractional transfer rate:

$$\text{Precipitate Removal Mass Flux} = \text{Precipitated Cell Mass} * \text{Transfer Rate}$$

The Transfer Rate has dimensions of inverse time. The Transfer Rate is specified as a scalar. That is, all precipitate species are transferred at the same rate.

In most applications, the Transfer Rate will simply be input either as a large number (such that any precipitated mass is immediately removed) or a function

that alternates between 0 and a large number (such that any precipitated mass is periodically removed, and allowed to accumulate between removals).

Precipitate removal mass flux links are uni-directional (mass can only be transported in one direction). That is, the Transfer Rate must be non-negative.

**Read more:** [Understanding Precipitate Removal Mass Flux Links](#) (page 107).

Note that in most cases, in order to use a Precipitate removal mass flux link you will need to specify a local solubility (a solubility that varies depending where you are in the model).

**Read more:** [Defining Spatially Variable Media Properties](#) (page 295).

### **Cell Pathway Example #5: Precipitate Removal Flux Links**

To illustrate the use of precipitate removal flux links, consider a simple case involving precipitation of a species from one Cell (a tank) to another Cell (representing a removal pond for sludge). This particular example file, Cell5\_PrecipitateRemoval.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

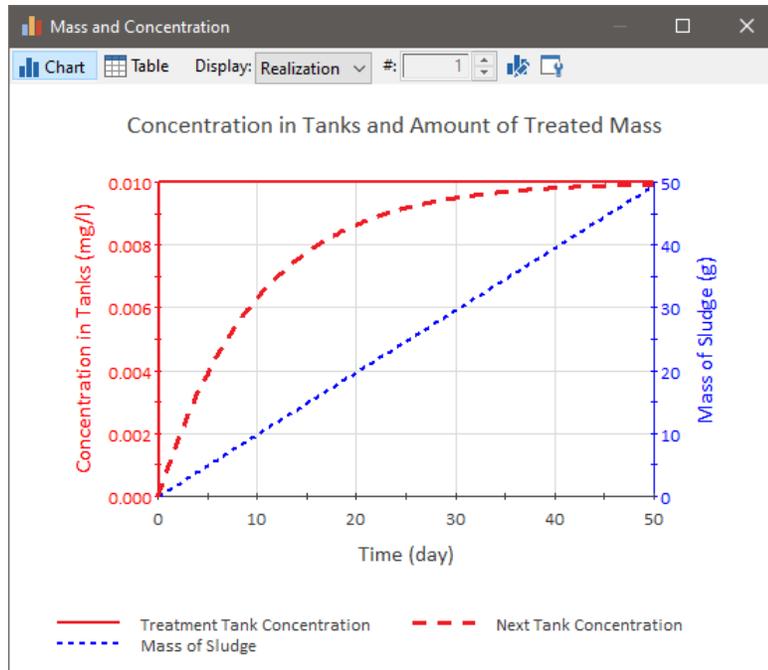
Suppose that the treatment tank contains 10 m<sup>3</sup> of water. Water cycles through the system at a rate of 1 m<sup>3</sup>/day (flowing to an equal sized tank). The incoming water contains Fe at a concentration of 1 mg/l (equivalent to a mass rate of addition of 1 g/day). Chemicals are added to the tank such that the Fe has a low solubility in the tank water (0.01 mg/l), causing it to precipitate out.

The precipitated solid is immediately collected (via a filter) and removed to a sludge tank. The treated water is then discharged to another tank, which subsequently discharges to a sink.

To simulate this system, you would do the following:

1. Define a single Species called Fe.
2. Specify a solubility of Fe in Water of 0.01 mg/l.
3. Create a Cell called Treatment\_Tank containing 10 m<sup>3</sup> of Water;
4. Define a Cell called Sludge containing 1 m<sup>3</sup> of water (the amount of Water is not important, as the Sludge Cell is simply acting as a sink for the precipitate);
5. Create a Cell called Next\_Tank containing 10 m<sup>3</sup> of Water;
6. Create a Cell called Sink (the amount of Water is not important, as it is simply acting as a sink);
7. Create an Input Rate for Treatment\_Tank equal to 1 m<sup>3</sup>/day \* 1 mg/l (equivalent to mass entering at a rate of 1 g/day);
8. Create an advective flux link between the Treatment\_Tank and the Next\_Tank with a flow rate of 1 m<sup>3</sup>/day.
9. Create an advective flux link between the Next\_Tank and the Sink with a flow rate of 1 m<sup>3</sup>/day.
10. Create a precipitate removal flux link between the Treatment\_Tank and the Sludge Cell with a high (100 day<sup>-1</sup>) transfer rate (so that the precipitate is removed immediately).
11. Specify the simulation settings (i.e., duration and timesteps), and run the model.

The output of this simulation, in the form of time histories of the concentration in the Next\_Tank and the amount of mass in the Sludge Cell is shown below:



Note that the concentration of Fe increases in the Next\_Tank (since it starts out empty), until it eventually approaches the concentration in the Treatment\_Tank (which never exceeds the solubility limit). The amount of precipitated mass that has been removed to the Sludge tank increases linearly at a rate of just under 1 g/day (nearly all of the Fe that enters the Treatment\_Tank precipitates, since it enters at a concentration of 1 mg/l, and the solubility limit is 0.01 mg/l).

## Treatment Flux Links to/from Cells

Treatment mass flux links are used to provide a mechanism for treating or removing a fraction of the amount of mass entering a Cell. They are defined by specifying a fraction of the mass entering the pathway which is removed. Hence, a treatment mass flux is computed as the mass rate of inflow of the species entering the pathway multiplied by a fraction:

$$\text{Treatment Mass Flux} = \text{Cell Mass Inflow Rate} * \text{Fraction}$$

The Fraction is dimensionless, and must be greater than or equal to 0 and less than or equal to 1. The Fraction is specified as a vector by species, which allows the Fraction to be species-specific.

Treatment mass flux links are uni-directional (mass can only be transported in one direction).



**Warning:** Treatment mass flux links only act on mass fluxes that are entering from outside the Cell net to which the Cell belongs. Hence, in order to filter incoming fluxes, they must be specified as Normal (as opposed to Coupled) flux links (or must be specified as direct inputs via the Cumulative Inputs field). Coupled influxes will not be impacted.

**Read more:** [Understanding Fraction of Inflows \(Treatment\) Mass Flux Links](#) (page 112).

## Cell Pathway Example #6: Treatment Flux Links

To illustrate the use of treatment flux links, consider a simple case involving removal of a two species from one Cell (a tank) before it flows to a second Cell (a second tank). This particular example file, Cell6\_Treatment.gsm, can be

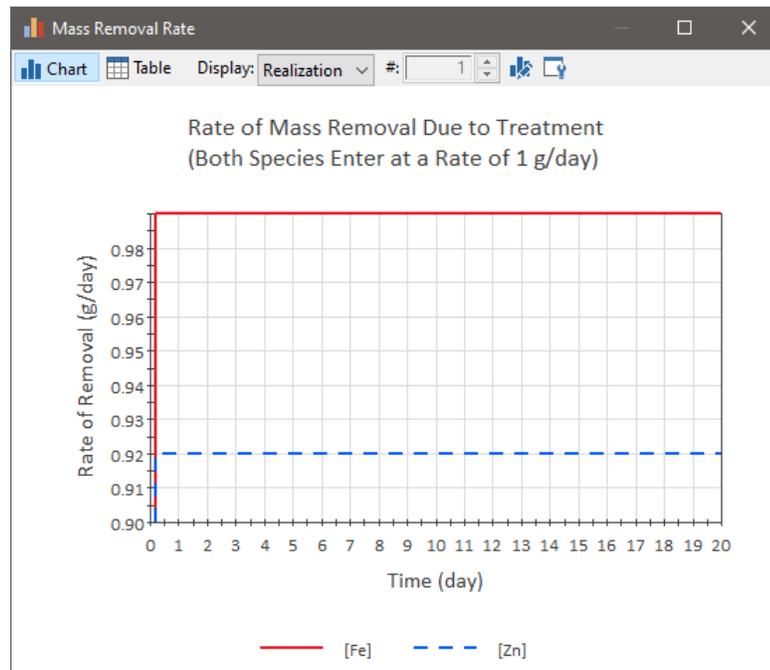
found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

Suppose that the tank contains 10 m<sup>3</sup> of water. Water cycles through the tank at a rate of 1 m<sup>3</sup>/day (flowing to an equal sized tank). The incoming water contains Fe at a concentration of 1 mg/l and 1 mg/l of Zn. A treatment process in the tank removes 99% of the Fe and 92% of the Zn.

To simulate this system, you would do the following:

1. Define two Species (Fe and Zn).
2. Create a Cell called Treatment\_Tank containing 10 m<sup>3</sup> of Water;
3. Create a Cell called Sink\_Downstream containing 1m<sup>3</sup> of Water (the amount of Water is not important, as this Cell is simply acting as a sink for the water leaving the Treatment\_Tank);
4. Create a Cell called Sink\_Mass containing 1 m<sup>3</sup> of Water (the amount of Water is not important, as this Cell is simply acting as a sink for the treated mass);
5. Create an Input Rate for Treatment\_Tank equal to 1 mg/l \* 1 m<sup>3</sup>/day for each species (equivalent to mass entering at a rate of 1 g/day);
6. Create an advective mass flux link between Treatment\_Tank and Sink\_Downstream with a flow rate of 1 m<sup>3</sup>/day.
7. Create a treatment flux link between the Treatment\_Tank and Sink\_Mass with the appropriate removal fractions; and
8. Specify the simulation settings (i.e., duration and timesteps), and run the model.

The output of this simulation, in the form of time histories of mass removal rate (the mass rate from Treatment\_Tank to Sink\_Mass) is shown below:



## Automatically Generating Cell Networks Using the CellNet Generator

Note that 0.99 g/day of Fe is removed, and 0.92 g/day of Zn is removed. Recall that the amount of mass entering the Treatment\_Tank is 1 g/day for each species.

In some situations, you may need to create a rectangular or cylindrical network of Cell pathways with advective and/or diffusive connections. Although such a network can be created manually, if it contains a large number of Cells doing so can become cumbersome and time-consuming. Therefore, GoldSim provides a special element to automate the creation of such Cell networks.

The CellNet Generator discretizes a rectangular or cylindrical region of space and creates a two-dimensional array of Cell elements, including any necessary advective or diffusive mass flux links between them. You can specify the existence of different fluid or solid materials in different parts of the generation region. If a fluid is defined, you can specify its flow velocity (the Darcy velocity, if a porous solid is defined). After defining the geometry of the region you wish to simulate, the level of discretization (i.e., the number of Cells), the properties of the Cells (i.e., the media they contain), and the nature of the advective and diffusive connections between the Cells, you instruct GoldSim to create the Cell network, and it automatically does so.

Once the Cell elements have been generated, you can manually edit them to add any flux links necessary to connect them to the rest of your model.

You insert a CellNet Generator element by selecting **Insert Element | Contaminant Transport | CellNet Generator** from the main menu or the context menu of the graphics pane.



**Note:** The Aquifer pathway also provides a way to automatically generate a Cell network. An Aquifer pathway performs its computations by creating a temporary Cell network during the simulation, which is subsequently removed at the end of the simulation. In most cases, there is no need for you to be aware of how this is done, or to view the temporary Cell pathways that are created. The Cell network generated by an Aquifer is always one-dimensional and homogeneous.

---

**Read more:** [Using Aquifer Pathways](#) (page 174).

---



**Warning:** The CellNet Generator is not intended to generate extremely large Cell networks (e.g., thousands of Cells). As the size of the network increases, the number of system resources required increases, and eventually the system will run out of resources and GoldSim will be unable to run.



**Note:** The CellNet Generator is only available within the RT Module. It is not available within the CT Module.

---

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4).

The details of using the CellNet Generator are provided in the sections below.

## Defining the Geometry of the Cell Network

The CellNet Generator property dialog looks like this:

CellNet Generator Properties : CellNet\_Gen1

Cell-net Definition

Element ID: CellNet\_Gen1 Appearance...

Description:

Cell-Net Definition

Length Unit: m Geometry: Planar Thickness: 1 m

X-direction: # Cells: 2 Start: 0 End: 10 Spacing: Regular

Y-direction: # Cells: 2 Start: 0 End: 10 Spacing: Regular

Create diffusive links

Zone Definition

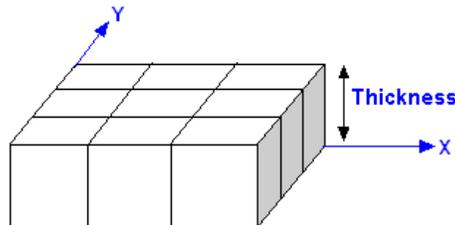
ID	Fluid	Vol.Frac.	Vx	Vy	Solid	Vol.Frac.	I
Zone1	-none-				-none-		-nt

Add Zone Remove Zone Map Cells... Generate Cells

OK Cancel Help

The first step in using the CellNet Generator to define the **Geometry** of the Cell net that you wish to generate. GoldSim provides two options for the geometry:

- **Planar:** The Cell net that is generated represents a rectangular region of specified **Thickness**. In this case, each Cell physically represents a rectangular prism:



- **Cylindrical:** The dialog takes on a slightly different appearance when you specify Cylindrical geometry:

CellNet Generator Properties : CellNet\_Gen1

Cell-net Definition

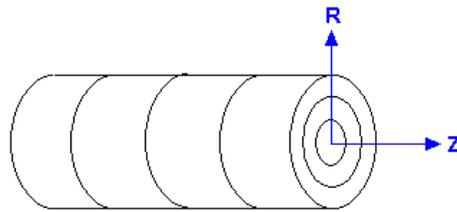
Length Unit: m Geometry: Cylindrical Angle: 360 deg

Z-direction: # Cells: 2 Start: 0 End: 10 Spacing: Regular

R-direction: # Cells: 2 Start: 0 End: 10 Spacing: Regular

Create diffusive links

The Cell net that is generated represents a cylindrical region that is axis-symmetric about the Z-direction. In this case, each Cell physically represents a cylindrical "shell":



By default, the Cell net represents a full cylinder (**Angle** = 360), but you can specify a smaller number (e.g., **Angle** = 180 would represent a half cylinder).

Note that all geometric data (e.g., thicknesses, angles) must be entered as numbers (not links).

After defining the geometry, you must next specify the level of discretization. **#Cells** defines the number of Cells in each dimension. **Start** and **End** specify the beginning and ending coordinates of the network in each dimension. They are specified without units, as they are assumed to be defined in the **Length Unit**. In most cases, **Start** will be specified as 0, and **End** will represent the length of the network in the specified direction.

The arrows adjacent to the direction control how the cells are created in the graphics pane. For example, if using planar geometry, and selecting the X-direction to go from left to right with 3 cells, and the Y-direction to go from bottom to top with 2 cells, GoldSim would generate 3 columns of 2 cells. Alternatively, if using planar geometry, and selecting the X-direction to go from top to bottom with 3 cells, and the Y-direction to go from left to right with 2 cells, GoldSim would generate 2 columns of 3 cells.

The following examples illustrate the use of the various fields to create specific geometries:

Cell-Net Definition									
Length Unit:	m	Geometry:	Planar	Thickness:	5	m			
X-direction:		# Cells:	2	Start:	0	End:	20	Spacing:	Regular
Y-direction:		# Cells:	2	Start:	0	End:	10	Spacing:	Regular
<input type="checkbox"/> Create diffusive links									

This would define a rectangular prism 20m long in the x direction, 10m long in the y direction and 5m thick. It would consist of a 2 x 2 grid of 4 Cells. Each Cell would be 10m long in the x direction, 5m long in the y direction, and 5m thick.

Cell-Net Definition									
Length Unit:	m	Geometry:	Cylindrical	Angle:	360	deg			
Z-direction:		# Cells:	4	Start:	0	End:	20	Spacing:	Regular
R-direction:		# Cells:	1	Start:	0	End:	2	Spacing:	Regular
<input type="checkbox"/> Create diffusive links									

This would define a one-dimensional cylinder, 20m long, with a radius of 2m. It would consist of a row of 4 Cells. Each Cell would represent a 5m long cylinder with a 2m radius.

Cell-Net Definition

Length Unit:  Geometry:  Angle:  deg

	# Cells:	Start:	End:	Spacing:
Z-direction:	<input type="text" value="4"/>	<input type="text" value="0"/>	<input type="text" value="20"/>	<input type="text" value="Regular"/>
R-direction:	<input type="text" value="5"/>	<input type="text" value="0"/>	<input type="text" value="5"/>	<input type="text" value="Regular"/>

Create diffusive links

This would define a 20m long cylinder, with a radius of 5m. It would consist of 20 Cells (4 columns of 5 cells). The cylinder would be divided into 4 equal-length (5m) sections. Each section would consist of a Cell (the first in each column) representing a central "core" cylinder (1 m radius), and 4 Cells representing concentric cylindrical shells (each having a thickness of 1m) around the core.

Cell-Net Definition

Length Unit:  Geometry:  Angle:  deg

	# Cells:	Start:	End:	Spacing:
Z-direction:	<input type="text" value="4"/>	<input type="text" value="0"/>	<input type="text" value="20"/>	<input type="text" value="Regular"/>
R-direction:	<input type="text" value="5"/>	<input type="text" value="5"/>	<input type="text" value="10"/>	<input type="text" value="Regular"/>

Create diffusive links

This would define a *hollow* 20m long cylinder, with an outer radius of 10m and a hollow center of radius 5m. It would consist of 20 Cells (4 columns of 5 cells). The cylinder would be divided into 4 equal-length (5m) sections. Each section would consist of 5 Cells representing concentric cylindrical shells (each having a thickness of 1m) around the hollow center. The innermost shell would be represented by the first cell in each column.

The **Spacing** field for each direction determines the spacing of Cells in each dimension. By default, the spacing is "Regular".

If "Length Ratio" is chosen, each successive Cell will be N times longer than the previous Cell, where N is the specified Ratio. For example, in this case:

	# Cells:	Start:	End:	Spacing:
X-direction:	<input type="text" value="3"/>	<input type="text" value="0"/>	<input type="text" value="7"/>	<input type="text" value="Length Ratio"/> <input type="text" value="2"/>

The first Cell would have a length of 1 unit, the second a length of 2 units, and the third a length of 4 units.

If "User-defined" is selected, an **Edit...** button appears:

	# Cells:	Start:	End:	Spacing:
X-direction:	<input type="text" value="10"/>	<input type="text" value="0"/>	<input type="text" value="50"/>	<input type="text" value="User-defined"/> <input type="button" value="Edit..."/>

Pressing this button provides access to a dialog for directly specifying the lengths of each Cell:

Define Axis

In each row specify the X-coordinate for the start of the corresponding Cell element.  
In the last row specify the X-coordinate for the end of the last Cell.

X1	0
X2	2
X3	4
X4	6
X5	8
X6	10
X7	12
X8	20
X9	30
X10	40
X11	50

OK  
Cancel  
Help

This defines the length of 10 Cells along the X-direction. The first 6 Cells have a length of 2m, the 7<sup>th</sup> Cell has a length of 8m, and the last three Cells have a length of 10m.

### Defining Property Zones Within the Cell Network

The bottom portion of the CellNet Generator dialog is used to define zones of different properties within the Cell network:

Zone Definition

ID	Fluid	Vol.Frac.	Vx	Vy	Solid	Vol.Frac.	
Zone1	Water		1 m/day	0.1 m/day	Sand		-nc
Zone2	Water		10 m/day	1.5 m/day	Gravel		-nc

< >

Add Zone Remove Zone Map Cells... Generate Cells

You can add and remove zones using the **Add Zone** and **Remove Zone** buttons, respectively. Each zone is given an ID (the default is Zone1, Zone2, etc.). These Zone IDs are incorporated into the names of the Cells that will be generated, so choosing the ID carefully is worthwhile.

**Read more:** [Creating the Cell Network](#) (page 158).

For each zone, you have the option to define a up to two **Fluids** and a single (porous) **Solid** from a drop-down list (which includes all the available media).

The **Vol. Frac.** for the Solid (the column immediately to the right of the Solid column) represents the fraction of the total Cell volume filled by the solid (porous) medium. If you have a Solid present, this will typically be 1. Hence, if you specify a Solid, and leave the Vol. Frac. empty, a value of 1 is assumed.

The **Vol. Frac.** for the first Fluid (the column immediately to the right of the Fluid column) represents the fraction of the remaining volume (accounting for any Solids present) that is filled with the first specified Fluid. Hence, if the Solid fills the entire volume, the **Vol. Frac.** for the Fluid represents that saturation fraction. If you leave the Vol. Frac. for a Fluid empty, a value of 1 is assumed.

**Vx** is the (Darcy) velocity for the first Fluid in the positive X-direction. **Vy** is the velocity in the positive Y-direction. GoldSim advective mass flux links actually require a flow rate (Q). Given a velocity, the flow rate is internally computed as  $V \cdot A$ , where A is the cross-sectional area perpendicular to the flow direction (and determined by the geometry specifications). Hence, if a porous medium solid is specified, **Vx** and **Vy** represent Darcy velocities.

For Cylindrical geometries, **Vx** becomes **Vz**, and **Vy** is replaced with **Qr**. **Qr** represents the total flow in the radial direction per unit length of the Z axis. **Qr**

must have units of Length<sup>2</sup>/Time. For example, to simulate a well with a screened length of 2.5 m and an inflow rate of 1 m<sup>3</sup>/day,  $Q_r$  would be specified as  $-1 \text{ m}^3/\text{day} / 2.5 \text{ m} = 0.40 \text{ m}^2/\text{day}$  (the value is negative because flow is in the negative R direction).

$V_x$  and  $V_y$  (and  $V_z$  and  $Q_r$ ) can be entered as equations, and can include links. If the links cannot be found when the Cell net is generated, the Cell net will still be created, but GoldSim will subsequently display error messages after the Cells are created, reporting that some of the inputs are invalid.

You can specify the direction of flow by using a negative sign in front of the definition for  $V_x$  and  $V_y$  (and  $V_z$  and  $Q_r$ ). During the creation of the Cell net, the negative sign is taken to mean that the flow is in the negative X, Y, Z or R-direction. The direction is implemented, and the negative sign is then removed. For example, if you specified the following:

ID	Fluid	Vol.Frac.	Vx	Vy	Solid	Vol.Frac.	I
Zone1	Water		- 1 m/day		Sand		-nc

GoldSim would create advective mass flux links that flowed from end to beginning in the row(s) of Cells that were created in the X-direction, with a flow rate of  $1\text{m/day} * \text{the appropriate area}$ . In this case, the “end” and “beginning” are relative to the directionality for the Cells defined when specifying the discretization. A positive flow is in the same direction as the arrow, and a negative flow is in the direction opposite to the arrow.



**Note:** Because the CellNet Generator can only automatically create advective flux links to other Cells in the net it is creating, any boundaries of a Cell net are no-flow boundaries.

The **Fluid2** column allows you to add a second Fluid to each Cell in the network. The second Fluid is assumed to fill any remaining pore space in the Cell (i.e., the first Fluid is assumed to be the wetting fluid). The  $V_x$  and  $V_y$  Darcy velocities only apply to the first Fluid (i.e., you cannot use a CellNet Generator to automatically create advective connections for both Fluids).



**Note:** If the Vol. Frac. for the first Fluid is specified as the *number 1* (or is left blank, which is equivalent to specifying a Vol. Frac. of 1), the second Fluid will not be added (since there is no remaining pore space to fill). However, if the Vol. Frac. for the first Fluid is specified as a link or expression, the second Fluid will be added to the Cells (even if the specified link is equal to 1, and the second Fluid therefore would have zero volume).

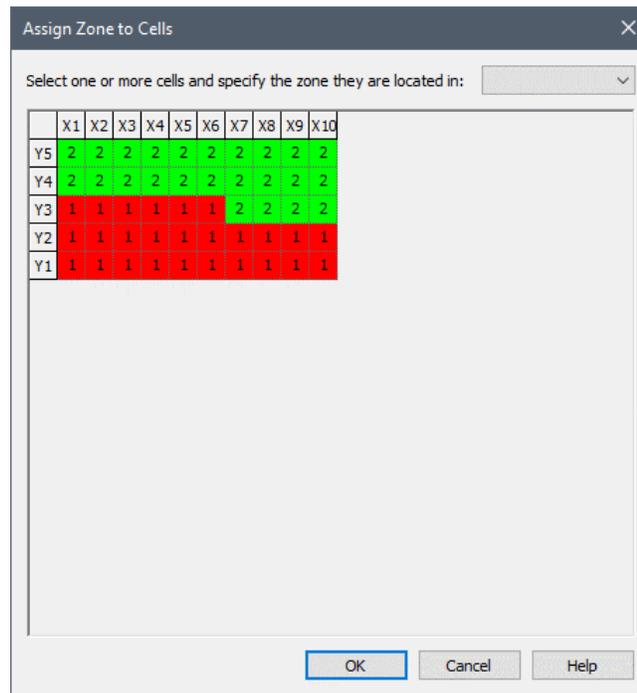
If you check the **Create diffusive links** checkbox, GoldSim will also create diffusive links between the cells. This also enables access to the last two columns in the Zone Definition section: **DFx** and **DFy** (**DFx** and **DFr** if cylindrical). These columns allow you to specify adjustment factors for diffusivities. These values (which should be dimensionless) multiply the diffusive areas between adjacent cells. This can be used to represent anisotropy in the diffusivity.

If you add a second Fluid (and the first Fluid has a Vol. Frac. less than 1), and you choose to create diffusive links, GoldSim will create diffusive links for both fluids. For example, to simulate diffusion within a partially saturated porous medium through both water and air, you would define the first Fluid as water

and the second Fluid as Air, and check the **Create diffusive links** checkbox. This would create a Cell net with both aqueous and gaseous diffusive links.

**Read more:** [Specifying a Cell Network with Partially Saturated Porous Media](#) (page 157).

After you have defined the zones, you must then map the zones onto each of the Cells you are creating. This is done by pressing the **Map Cells...** button, which displays the following dialog:



This dialog is a schematic two-dimensional plot of the cell network.

By default, all Cells are assigned to the first zone. To assign one or more Cells to a different zone, select the Cells by dragging the mouse over the Cells to select them, and then select the appropriate zone from the drop list at the top of the dialog.

### **Specifying a Cell Network with Partially Saturated Porous Media**

The CellNet generator can be used to create a Cell net representing a partially saturated porous medium system. In most cases, this will be a system that is partially saturated with water (with the second fluid being air).

To create such a system, you must:

- Specify a Vol. Frac. (i.e., saturation) for the first Fluid of less than 1; and
- Specify a second Fluid (in the **Fluid2** column).

In most cases, the first Fluid will be water, and the second Fluid will be air.

The second Fluid is assumed to fill any remaining pore space in the Cell (i.e., the first Fluid is assumed to be the wetting fluid).

By specifying Darcy velocities when defining the zones, the CellNet will create advective connections in the first Fluid (typically water).

If you check the **Create diffusive links** checkbox, GoldSim will create diffusive links for *both* fluids. That is, if you defined the first Fluid as water and the

second Fluid as Air, GoldSim would create a Cell net with both aqueous and gaseous diffusive connections.



**Note:** To accurately simulate diffusion through partially saturated porous media, it is important that you define a Diffusive Reduction Formula for each Fluid that varies with saturation. Note that when automatically generating diffusive connections using a CellNet Generator, the saturation level for the fluids is defined directly by the user (via the Vol. Frac. input), as opposed to being computed internally by GoldSim as a function of specified volumes.

**Read more:** [Diffusion Through Partially Saturated Porous Media](#) (page 142).

## Creating the Cell Network

Once you have defined the geometry, discretization and zone properties for your Cell network, you are ready to instruct the CellNet Generator to create the Cells. Before doing so, you must complete one final step:

- Specify whether or not you wish to **Create diffusive links**. If the **Create diffusive links** checkbox is cleared, only advective mass flux links between the Cells will be created. If the **Create diffusive links** checkbox is checked, diffusive mass flux links are created between all adjacent Cells.



**Note:** As is the case for advective flux links, diffusive flux links can only be created in the X and Y (or Z and R) directions. Diagonal links are not created.



**Note:** If  $V_x$  and  $V_y$  are empty for all zones, no advective mass flux links will be created.

Once you have completed this step, you create the Cell network by pressing the **Generate Cells** button. The Cells are created in the same Container as the CellNet Generator element, and are named as follows:

ZoneID\_cc\_rr

where *ZoneID* is the name of the Cell's zone, *rr* is the "row number", starting from the lowest Y (or R) direction value, and *cc* is the "column number", starting from the lowest X (or Z) direction value.

For example, if the geometry was defined as follows:

		# Cells:	Start:	End:	Spacing:
X-direction:		3	0	15	Regular
Y-direction:		2	0	10	Regular

and all Cells were in a single zone (with a ZoneID of ABC), the Cell network that would be created would look like this:



Note that the first row is the bottom row (since the Y-direction was specified to be from bottom to top), and the first column is the left-most (since the X-direction was specified to be from left to right).

GoldSim inserts the dimensions of the Cell in the Description field for the Cell. For example, for Planar geometry, the Description for ABC\_X1Y2 would look like this:

Element ID:	ABC_X1Y2	Appearance...
Description:	x-length = 5m, y-length = 5m, thickness = 1m.	

All of the necessary Media quantities (volumes and masses) and mass flux link properties are automatically generated and inserted into the appropriate fields of the Cell property dialogs.

Once the Cells have been generated, you will need to manually add any required boundary conditions and mass flux links to connect the network to other pathways and elements in your model.

## Simulating Solubility Limits in Cells

One of the most powerful features of Cell pathways is that you can impose a solubility constraint within them. Solubility limits are defined for each species within Fluid elements.

**Read more:** [Reference Fluid Properties](#) (page 65); [Fluid Properties](#) (page 69).

The solubility represents the maximum dissolved concentration that the species can have within a Fluid in a Cell.



**Note:** If a Fluid contains suspended particulates, the effective concentration could exceed the solubility limit, since the effective concentration includes the effect of the species mass associated with the suspended solids. In fact, for low solubility species, the species mass associated with suspended Solids could be the most important contributor to the effective concentration.

When a solubility constraint is applied for a species in a Cell, the Cell has a *saturation capacity* with respect to that species, which represents the maximum amount of species mass the Cell can contain before the species mass will start to precipitate out of solution.

The saturation capacity of a cell is a function of the solubility limit, the partition coefficients for the other media present in the cell, and the quantities of the media present in the cell:

$$msat_i = sol_i \sum_{g=1}^{NM} K_{gi} \cdot VM_g$$

where:

- $msat_i$  = saturation capacity for species  $i$  in the cell [M];  
 $sol_i$  = solubility of species  $i$  in the Reference Fluid [M/L<sup>3</sup>];  
 $K_{gi}$  = partition coefficient between medium  $g$  and Reference Fluid for species  $i$  [(L<sup>3</sup>/L<sup>3</sup>) for Fluids or (L<sup>3</sup>/M) for Solids];  
 $VM_g$  = quantity (volume or mass) of medium  $g$  in cell [L<sup>3</sup> for Fluids or M for Solids]; and  
 $NM$  = the number of media in cell.

If the total species mass in the Cell does not exceed the saturation capacity, the solubility limit has not been reached, and concentrations in the various media in the Cell are computed based on partition coefficients and media quantities.

**Read more:** [Understanding Partitioning in a Cell](#) (page 125).

If, however, the saturation capacity is exceeded, media concentrations are computed differently. In particular, the concentration in the Reference Fluid (if it is present) is set to the solubility limit, and the concentrations in other media are computed based on their partition coefficients and the concentration in the Reference Fluid. In addition, the concentrations in Solids in the Cell are incremented by the amount of "precipitated" species mass (the difference between the total mass in the Cell and the saturation capacity).



**Note:** You can track the amount of precipitated mass in a cell by checking the **Output Precipitated Mass** checkbox at the bottom of the cell dialog. If you do so, a new output (Precipitated\_Mass) is added to the cell.

**Read more:** [Cell Pathway Outputs](#) (page 133).

Mathematically, this can be restated more precisely as follows:

- The concentration in the Reference Fluid is set to the solubility limit for species  $i$ ,  $sol_i$  [M/L<sup>3</sup>];
- The concentration [M/L<sup>3</sup>] in all other Fluids ( $c_{fi}$ ) is computed as:

$$C_{fi} = sol_i K_{fi}$$

where  $K_{fi}$  is the partition coefficient for the species in fluid  $f$  [dimensionless].

- The concentration [M/M] in *suspended (particulate)* Solids ( $c_{pi}$ ) is computed as:

$$C_{pi} = sol_i K_{pi}$$

where  $K_{pi}$  is the partition coefficient for the species in suspended Solid  $p$  [L<sup>3</sup>/M].

- The concentration [M/M] in Solids *which are not suspended* ( $c_{si}$ ) is computed as:

$$c_{si} = sol_i K_{si} + \frac{(mtot_i - msat_i)}{\sum_{s=1}^{NS} VM_s}$$

where  $K_{si}$  is the partition coefficient for the species in Solid  $s$  [ $L^3/M$ ],  $mtot_i$  is the total mass in the cell [ $M$ ],  $msat_i$  is the saturation capacity [ $M$ ],  $VM_s$  is the mass of (non-suspended) Solid in the Cell, and  $NS$  is the number of non-suspended Solids in the Cell.

Note the difference between the treatment of suspended Solids and those that are not suspended. In particular, for computational reasons, the mass in the cell in excess of the saturation capacity (the "precipitated" mass) is assumed to be precipitated only onto those Solids which are not suspended. Hence, although species mass can be partitioned onto (and transported with) particulate Solids, *precipitated* species mass is never associated with suspended Solids.



**Note:** A medium that has zero volume (Fluids) or mass (Solids) cannot have a species concentration. Any mass in the Cell will partition into other Fluids or Solids and precipitated mass will become associated with any (non-suspended) Solids present in the Cell (proportional to the mass of each Solid).



**Note:** GoldSim provides a special mass flux link that allows you to selectively remove precipitated mass from a Cell.

**Read more:** [Understanding Precipitate Removal Mass Flux Links](#) (page 107).

If you are simulating multiple isotopes of the same element, GoldSim must handle the solubility calculations in a special way. This is because, physically, solubility is actually an element property (as opposed to an isotopic property).

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).

Therefore, GoldSim does the following:

1. It assumes that the solubility entered for the first isotope of the element in the species list is the element solubility;
2. It uses the sum of the mass (actually, the moles) of all isotopes of an element to determine if the elemental saturation capacity has been exceeded; and
3. If the elemental saturation capacity has been exceeded, it "shares" the elemental solubility in the Reference Fluid among the isotopes of the element based on the isotopic ratios. (For example, if the uranium isotopes  $^{235}\text{U}$  and  $^{238}\text{U}$  were present in a Cell at an isotopic ratio of 2 to 1, and the total mass of uranium in the Cell exceeded the saturation capacity, the dissolved concentration of  $^{235}\text{U}$  would be computed as 2/3 of the elemental uranium solubility.)

**Read more:** [Understanding Solubility Calculations](#) (page 167).



**Warning:** Solubility limits are not applied in Cells with a Defined Concentration boundary condition. If the Defined Concentration for a species is above the solubility limit, the solubility limit is ignored, the Defined Concentration is applied, and a warning is written to the Run Log.

**Read more:** [Defining Initial and/or Boundary Conditions for a Cell](#) (page 126).



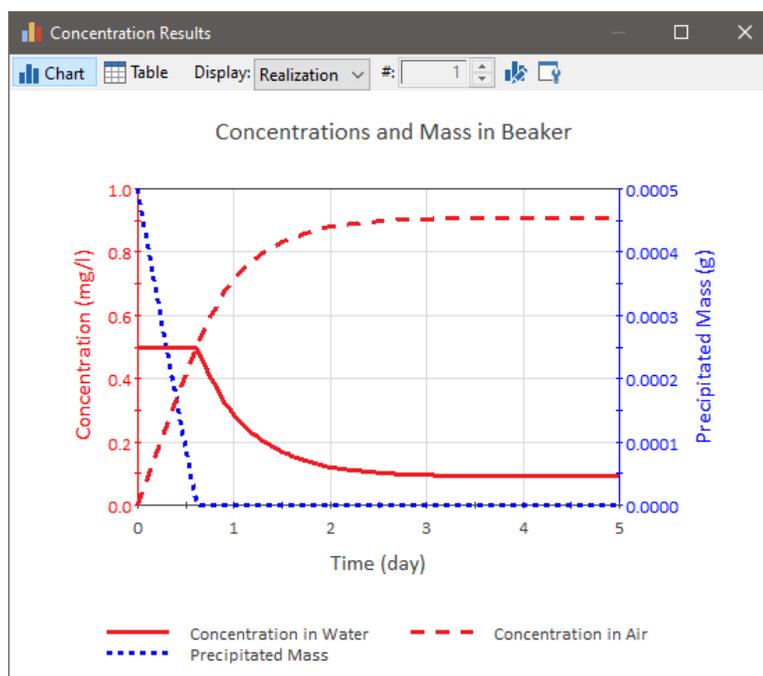
**Warning:** The “turnover rate” for a species in a Cell is defined as the ratio of the discharge rate for the species to the current amount of species in the Cell. The product of the turnover rate and the timestep indicates how many times the Cell is “flushed” within one timestep. If this product is very high, due to round-off error the species could oscillate between a saturated and unsaturated condition, which can cause the solution to slow down considerably. To prevent this, if the turnover rate multiplied by the timestep exceeds 1000 (implying that in one timestep, the Cell flushes its mass on the order of 1000 times), solubility limits are no longer applied (for all species). The fact that this occurs is written to the Run Log (but it is not treated as a Warning or Error, so that you will not be notified). Note that if the turnover rate varies dramatically, application of solubility limits may be activated and deactivated multiple times during a simulation. However, only the first instance is written to the Run Log.

### Cell Pathway Example #7: Solubility Constraints

To illustrate the use of solubility constraints, we can reconsider Cell Pathway Example #3, which simulated a volatile chemical diffusing across an air-water interface. The only change we will make is to add a solubility constraint (of 0.5 mg/l) for the chemical in water. This particular example file, Cell7\_DiffusionSolubility.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

**Read more:** [Cell Pathway Example #3: Diffusive Flux Links](#) (page 144).

The output of this simulation, in the form of time histories of the concentrations of the organic in both Cells, is shown below:



This chart also show the amount of precipitated mass in the Cell.

Note that the concentration in the Water is initially held constant at the solubility limit, implying that the saturation capacity of the cell is exceeded. During this time period, the concentration in the air increases linearly, since the concentration difference is essentially constant (0.5 mg/l minus a very small

## Coupling a Network of Cell Pathways to a Network of Reservoir or Pool Elements

number). Also during this time, the amount of precipitated mass decreases linearly. After about a half of a day, the water cell is no longer saturated (since sufficient mass has diffused out of the "Water\_Side" Cell), the concentration falls below the solubility limit, and the amount of precipitated mass goes to zero.

The Contaminant Transport Module is a mass transport model. That is, it tracks the mass of the species as it moves them through the pathway network. However, GoldSim does not automatically impose a mass balance on the transport media that it is moving between pathways (e.g., water). Mass balances for transport media must be specifically imposed by the user.

In practice, this simply means that when specifying the media amounts (typically volumes of water) and media flow rates for Cells (and other pathways), you must be careful to ensure that there is a flow balance. For some systems, ensuring a flow balance may be quite straightforward. For example, if the Cells represented portions of a saturated aquifer, the volume of water in each Cell remains constant, and you need to only ensure that the flows between Cells are consistent. In many cases, you may not even require a separate calculation for the flow rates, as they may be simply specified (or perhaps read from a Time Series).

However, if your Cells represent surface water bodies, or other compartments in which the quantity of media (e.g., water) varies with time, then you will need to build a parallel calculation in your model that tracks the water balance. This will almost always be done using Pool or Reservoir elements (discussed in "Pool Elements" and "Reservoir Elements" in the **GoldSim User's Guide**).

In this case, it is necessary to couple the network of Pool or Reservoir elements (representing the flow system) to the network of Cells (representing the mass transport system). This can be done as follows:

- The Amount of each medium in a Cell (e.g., water) should be defined using the corresponding element (e.g., a Reservoir or Pool) that is being used to track that medium:



Cell Pathway Properties : Pond

Definition | Inflows | Outflows | Diffusive Fluxes

Element ID: Pond Appearance...

Description:

Media in Cell

Medium	Amount	F	H	S
Water	Volume	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Add Medium Delete Medium

Cell Inventory

Initial Inventory:

Discrete Changes:  +

Save Masses in Pathway

Output Precipitated Mass

Final Values  Time History

OK Cancel Help

- The Outflow Flow Rates for each Cell should be defined using the appropriate rates for the corresponding element (e.g., outflow/withdrawal rates and/or overflow rates associated with a Reservoir or Pool).



**Note:** It is highly recommended that you use Pools, rather than Reservoirs when building a flow network that will link to a Cell network. This is because Pools have a number of distinct advantages (in particular, they have separate output for each outflow and they have total inflow and total outflow outputs) that make the coupling process much simpler.



**Warning:** If the media amounts (e.g., volumes of water) within your flow system (that you are modeling using Reservoirs or Pools and linking to Cells) change very rapidly over a timestep or go to zero (e.g., due to evaporation), Cells can compute incorrect concentrations and mass transfer rates. In these cases, GoldSim will write warning messages to the Run Log, and there are actions you can take to minimize such errors.

---

**Read more:** [Dealing with Changing Media Amounts in a Cell](#) (page 169).

## Basic Concepts of the Cell Solution Algorithm

The algorithm used by GoldSim to compute concentrations and fluxes associated with Cells is discussed in detail in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

Although it is not necessary for you to understand the details of this algorithm in order to use Cells in your models, there are several situations in which at least a basic understanding of the Cell solution algorithm is necessary in order to maximize the computational efficiency of your model and the accuracy of the results.

## Understanding How Cells Manage Flow Balance

The quantity of a medium in a Cell is specified directly by the value in the media list for the Cell. It is important to understand that these values are not changed by the specified Outflows and/or Inflows of that medium from/to the Cell. That is, even though you specify the rate at which the medium leaves (and/or enters) the Cell when you create an advective flux, this has no affect the quantity of the medium in the Cell(s). GoldSim uses the advective rates only to transport mass and does not keep track of the movement of media (e.g., Water) through the pathway network.

So if you have specified that the quantity of medium is constant, but the Inflows are different than the Outflows, what does it mean and how does GoldSim treat this? The answer is that the specified volume is always respected. Conceptually, this implies that a quantity of "clean" medium (containing no species mass) enters (or leaves) the Cell in exactly the correct amount such that the quantity of medium in the Cell remains constant. For example, if a Cell had an Outflow flux link of Water of 10 m<sup>3</sup>/sec and Inflow flux link of Water from another Cell of 3 m<sup>3</sup>/yr, GoldSim would then assume that 7 m<sup>3</sup>/yr of "clean" Water also flowed into the Cell in order to conserve the Cell's volume.

If the volume in a Cell is constant, but the specified Outflows are greater than the specified Inflows (as in the example above), the effect on the species concentrations in the Cell is essentially one of dilution, since "clean" medium is assumed to be flowing into the Cell. If, however, the specified Outflows are less than the specified Inflows, the effect would be to *concentrate* mass in the Cell,

since GoldSim would assume that a quantity of "clean" medium (carrying no species mass) flowed *out* of the cell in order to conserve the Cell's volume. Although there are some physical situations in which you may actually want to do this (e.g., in order to simulate the evaporation of Water from a Cell), typically such behavior would not be intended. As a result, if during a timestep the Inflows to a Cell exceed the Outflows, and the quantity of the Reference Fluid is defined in such a way that it cannot change with time (e.g. using a Data element), GoldSim writes a (non-fatal) warning message to the Run Log to alert you to this.



**Note:** Although this is a helpful warning, every model you build will have at least one Cell in which the Inflows exceed the Outflows. This is because all models have an "edge" or an "sink" where the model ends, and you are no longer tracking mass. Hence, to avoid the warning message in this case, if the name of the Cell starts with the letters "sink" (case-insensitive), GoldSim will not issue the warning message for that Cell.



**Note:** The warning message is only written for the Reference Fluid. If the Inflows to a Cell exceed the Outflows for any other medium in the Cell or the quantity.

---

Of course, in some cases, the quantities of media in the Cell may actually be changing (e.g., the Outflows are greater than the Inflows, and no "clean" water is entering, and hence the Cell volume is decreasing). In such a case, you should explicitly represent this by modeling the flows and volumes (typically using Reservoir or Pool elements) and coupling this to the Cells (e.g., the amount of Water in the Cell would be defined as the output of a Reservoir or Pool).

**Read more:** [Coupling a Network of Cell Pathways to a Network of Reservoir or Pool Elements](#) (page 163).

---



**Note:** If the Inflows to a Cell exceed the Outflows, and the quantity is specified as being able to change with time (e.g., it is represented using a Reservoir or a Pool), GoldSim does not write a warning message to the Run Log to alert you to this. In this case, it is assumed that you are properly tracking the quantity directly.

---

## Understanding Cell Nets

When Cells are linked together via coupled mass flux links, GoldSim treats the network of Cells as a single coupled system of differential equations, solving for the mass of each species in each medium in each Cell as a function of time.

In order to solve these equations, GoldSim initially identifies the sub-networks of interconnected Cells, referred to as cell nets, which then are treated as single entities in the calculations. GoldSim sets up and solves a separate set of fully coupled equations for each net. Hence, the fluxes between cells *within* a cell net are computed simultaneously (since they are solved as a system of coupled differential equations). Fluxes *between* cell nets (or between cell nets and non-Cell pathways), however, are propagated asynchronously (i.e., the "upstream" pathway or cell net is solved first, followed by the "downstream" one).

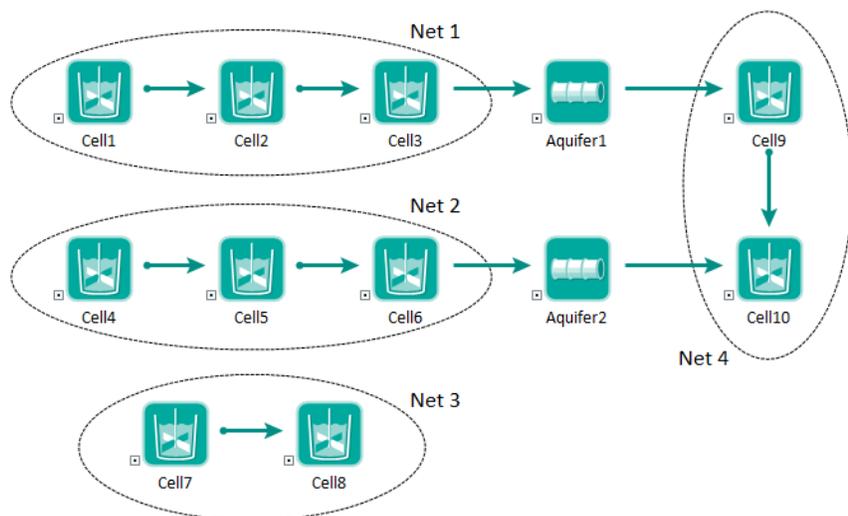
A cell net is defined by all Cells interconnected via coupled mass flux links. Note that since only Cell to Cell mass flux links can be coupled, two Cells

which are linked via mass flux links but are separated by a non-Cell pathway (e.g., a Pipe), are, by definition, in different cell nets. Also, if two Cells are connected by normal mass flux links (rather than coupled links), they will be in different cell nets.



**Note:** Cell nets cannot cross between SubSystems. A SubSystem is a specialized Container in GoldSim that is entirely self-contained. Hence, by definition, Cell nets cannot extend across a SubSystem boundary. SubSystems are discussed in Chapter 4 of the **GoldSim User's Guide**.

The example below shows a pathway network in a Container, illustrating schematically how GoldSim would define the cell nets.



*There are four cell nets in this Container. Cells in a cell net are all connected by coupled links, which are distinguishable from other types of links by the way their influences are drawn (i.e., they have a small circle at the beginning of the influence).*

In general terms, a transport pathway can be thought of as a function whose input is a mass rate, and whose output is a mass rate. This statement is not strictly true for all types of pathways. In particular, the statement is true for non-Cell pathways, but is not strictly true for Cell pathways (since mass transfer to or from a Cell with diffusive connections would not necessarily be unidirectional). It is, however, true for *cell nets*. Hence, each cell net can be thought of as a very complex sort of pathway, which acts as a transfer function having multiple unidirectional input and output connections.

The equations GoldSim solves for each net are defined in terms of *nodes*, where a node represents either a Cell in the cell net (primary nodes) or monitored discharges from the net (secondary nodes). GoldSim defines a secondary node for any mass flux link for which it needs to compute a flux rate:

- mass flux links to non-Cell pathways or to other cell nets;
- mass flux links within a cell net for which the user has requested that results be saved; and
- mass flux links which are referenced in other elements (e.g., Sum or Extrema) for which the user has requested that results be saved.

GoldSim solves a matrix equation representing the coupled system of equations based on the backwards-difference (fully implicit) algorithm for each cell net and each species decay-chain family to compute concentrations and fluxes. GoldSim uses an iterative, sparse-matrix approach (the bi-conjugate gradient stabilized method) to solve the system of equations.

The backwards difference (fully implicit) algorithm has the advantages of being unconditionally stable, conserving mass, and having bounded error levels. In order to enhance the accuracy of the backwards-difference method, GoldSim automatically divides every time step into a number of *fractional timesteps*, depending on the user's selected precision level (1 for Low, 4 for Medium and 10 for High). Other solution parameters (e.g., the overall solver error tolerance, as well as a minimum number of solver iterations, how solubility constraints are represented) are also determined by the precision setting.

**Read more:** [Understanding the Solution Precision](#) (page 247).

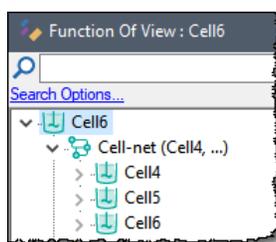
Using fractional timesteps is a very computationally efficient way to enhance the accuracy of the solution. This is because 1) only the cell nets are updated during these fractional timesteps; and 2) numerically the fractional timesteps are computed via matrix calculations in such a way that it takes less computational effort than simply shortening the actual timestep. However, fractional timesteps can also have a detrimental affect (i.e., produce inaccuracies) when the media amounts (e.g., the volume of water) is rapidly changing in a Cell. In these cases, GoldSim will write warning messages to the Run Log, and there are actions you can take to minimize any errors.

**Read more:** [Dealing with Changing Media Amounts in a Cell](#) (page 169).

The computational effort to solve the coupled equations of a cell net increases rapidly (i.e., not linearly) with the size of the cell net. In almost all models, this is not a problem, but for extremely large models (hundreds of Cells), it may be worthwhile to break a very large cell net into several smaller cell nets (by using a Normal link in place of a Couple link when connecting Cells).

**Read more:** [Specifying the Link Type for Mass Flux Links](#) (page 118).

Note that because cell nets are computationally treated as a single entity, they are presented as such in the Function of and Affects view:



*In the Function of or Affects View, a cell net is identified by its first member. For example, the cell net containing Cell4, Cell5, and Cell6 is referred to as "Cell-net (Cell4, ...)"*

## Understanding Solubility Calculations

GoldSim uses the backwards difference (fully implicit) algorithm to integrate the cell matrix equations over time. The resulting matrix equations are solved using an iterative, sparse-matrix solution algorithm (a preconditioned conjugate gradient approach, described further in Appendix B of the Contaminant Transport User's Guide). The backwards difference algorithm has the advantages of being unconditionally stable, conserving mass, and having bounded error levels. GoldSim automatically uses fractional timesteps (based on the user's 'solution precision' selection) in order to control the accuracy of the results. In

general, users can rely on GoldSim to compute accurate results, with the accuracy controlled by the 'solution precision' choice.

Note, however, that the equations for a cell net change when a species reaches its solubility limit in a Cell. GoldSim monitors concentrations in the Reference Fluid. If the concentration for a species reaches the solubility limit, GoldSim applies a boundary condition, holding the dissolved concentration in the Reference Fluid at the solubility limit, and switches to the solubility-limited (saturated) form for the matrix equations.

After switching to the solubility-limited (saturated) equations, GoldSim monitors the total mass of the element in the Cell. If this ever falls below the amount needed to reach the solubility limit, GoldSim switches the equations back to their standard form.

To carry out these processes with precision, GoldSim automatically uses a search algorithm to find the exact point in time where the governing equations change and then dynamically adjust the timestep to a value which can be much shorter than the user-specified timestep. These *substeps* (which are determined by the selected Solution Precision) can be as small as 1e-8 times the actual timestep length. Note that the substeps are used only when computing cell nets, and are not applied to elements outside of cell nets.

**Read more:** [Understanding the Solution Precision](#) (page 247).

Using the search algorithm, GoldSim does the following:

1. It attempts to identify the exact point in time at which a species (or element) changes its saturation state to or from saturated. The search succeeds if the "overshoot" across the solubility limit is less than a specified fraction of the limit. If the overshoot exceeds this, the substep is reduced. This is repeated until the overshoot is less than the specified tolerance, or a minimum substep is reached. The overshoot tolerance and the minimum substep are determined by the Solution Precision.
2. It checks that the relative fractions of isotopes of a saturated element do not change excessively during a timestep. Similarly to changing the solubility state, GoldSim carries out a search in time trying to limit the change in isotopic fractions to a specified fraction of the value when the boundary conditions were last calculated. This fraction is determined by the Solution Precision. (This check is only carried out for isotopes present in the Cell in quantities greater than 1 $\mu$ g AND representing more than 1% of the total element mass).
3. It checks for a condition where an initially saturated species or element discharges mass at such a high rate that even at the shortest possible substep it calculates a negative remaining mass (of more than 1 $\mu$ g) in the cell at the end of the timestep. If the amount of mass in the Cell is negative at the end of the substep, GoldSim sets it to zero (*which has the effect of creating mass in the system*, as the "downstream" pathway will still retain the mass it received), and records a warning message in the Run Log.



**Note:** The cell net solution algorithm (including the values for the various parameters for the different Solution Precision options) is discussed in detail in Appendix B (in a section entitled *Solving the Matrix Equations Numerically*).

---

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

If the internal rates of mass transfer are high and/or the timestep is too large, the search algorithm may fail to converge to within the tolerance limits even using the shortest allowable substep. If this occurs, warning messages are written to the Run Log. The warning will state that "**smallest substep failed**" along with the time, the Cell involved, the species involved, and the error code. There are four error codes:

- The "unsat - sat" and "sat - unsat" error codes indicate that there was an unacceptable "overshoot" across the solubility limit from below or above, respectively. "sat-unsat" errors are unlikely to have significant impacts on results (since they simply imply that an element was held at the solubility limit for a fraction of a timestep longer than it should have been). An "unsat-sat" error (in which the solubility limit is overshoot from below), however, can result in a one timestep "spike" in which the solubility limit is unrealistically exceeded for the specified element. Unless this is for a key species in the simulation, however, in most cases this will not have a large impact on results.
- The "overshoot" error code indicates that the isotopic fractions changed to an unacceptable degree during the timestep. This error is often incurred when isotopes with very short half-lives exist in the system, and unless those isotopes are key species, it is unlikely to have significant impacts on results.
- The "negative inventory" error code is an extreme case of the "sat-unsat" error and indicates that more mass was discharged from the cell than it contained. This results in a negative mass in the cell. GoldSim subsequently resets this to zero, which has the impact of creating mass in the system. This is the most extreme type of error that can occur, and GoldSim therefore warns the user that "**erroneous mass was created**". GoldSim also sums and reports the total amount of mass that was created.



**Note:** GoldSim can print additional details that can be useful for evaluating these error messages. To do so, check the **Log cell-network details** checkbox in the **Contaminant Transport** tab of the **Options** dialog.

---

If any of these errors occur (particularly the "negative inventory" error), and the impact on the simulation is likely to be significant, you should do the following (in this order) until the problem is resolved:

1. Check to see if some mass transfer rates have been specified as being unrealistically large (e.g., a Cell "flushing" mass out very rapidly) and correct this if you find it (i.e., flush mass from Cells more gradually).
2. Repeat the run using a higher precision level.
3. Repeat the run using a smaller value for the GoldSim timestep.

### **Dealing with Changing Media Amounts in a Cell**

If the quantity of the medium involved in advecting mass (typically the volume of water) in a Cell is constant or changing slowly, the solution algorithm is quite accurate. However, rapidly changing Cell media amounts can result in errors in computed concentrations (and mass transfer rates).

These errors are most common and significant when the amount of media in a Cell is low and rapidly changing (either emptying or filling), in which case the fractional volume change is by definition high. In this case, computed

concentrations in a Cell can show unrealistic jumps or drops (i.e., positive or negative “spikes”). These can, in turn, result in inaccurate mass transfer rates and can therefore propagate downstream producing additional inaccurate behavior. The errors will be small as long as the amount of media does not change significantly (e.g., > 10 or 20%) over a full timestep, but can become significant if it does.

If a Cell completely empties (the media amount goes to zero), an additional problem occurs. In particular, when a Cell empties, some mass will be left in the Cell after it has emptied. More importantly, if the Cell is empty but still has an inflow (with a matching outflow), mass will accumulate in the Cell. If the Cell then refills, any mass left behind (or accumulated) in the Cell would be released suddenly (and this itself could result in unrealistic spikes).



**Note:** Of course, if the Cell emptied at least partially due to evaporation (which would not be unusual, for example, for a surface water body that went dry), some mass realistically would in fact be left behind in the Cell, since evaporation does not transport mass (and mass would eventually precipitate out of solution as water evaporated). The discussion above, however, refers to the fact that even if the Cell empties due to outflows that transport mass (and there is no evaporation), mass will be (unrealistically) left behind for numerical reasons.

To keep this problem in perspective, however, it should be noted that in the real-world, the behavior of solutes in a system in which a Cell was emptying would likely be very complex, and hence very difficult to model accurately. This is because the processes controlling concentrations as a Cell empties are often difficult to accurately represent. In particular, in many cases, as pointed out above, one of the key outflows for a Cell that is emptying (e.g., a pond) would be evaporation. In such a case, solutes would precipitate out of solution before the Cell emptied (and the geochemistry of such a high concentration solution would be quite complex indeed).



**Note:** Numerically, these two problems arise for two different reasons. The error associated with mass being left behind in an empty Cell is a direct outcome of using an implicit approach to solve the equations. The error associated with rapidly changing Cell volumes is a result of the fractional timestep algorithm implemented by GoldSim (which improves accuracy under most conditions, but can produce erroneous concentrations with rapidly changing media amounts). A detailed explanation of why these problems arise is provided in Appendix B (in the sections entitled *Solving the Matrix Equations Numerically* and *Minimizing Errors for Systems with Rapidly Changing Media Amounts*). These sections also provide a more detailed explanation of the two methods presented below for addressing these problems.

---

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

If the conditions that can lead to either of these two problems occur, a warning message will be written to the Run Log. In particular, GoldSim monitors the volume of the Reference Fluid and writes a warning message if this is changing in such a way that it could cause erroneous results. It also writes a (separate) warning if the amount of any media (typically the Reference Fluid) goes to zero.



**Note:** The warning message associated with rapidly changing media amounts is only written for the Reference Fluid. It is not written if other media are changing rapidly.

Fortunately, when these problems do arise, their impact can be minimized. There are two different approaches for doing so.

#### Approach 1: Run Using Low Precision

One approach is to simply use Low Precision when running the model. As pointed out above, the error associated with rapidly changing Cell media amounts is a result of the fractional timestep algorithm implemented in GoldSim. This algorithm, however, is not used for Low Precision runs. As a result, the “spiky” behavior will not manifest itself. (In fact, if you run at Low Precision, GoldSim will not produce the warning message mentioned above resulting from rapidly changing Reference Fluid volumes).

However, the problem associated with leaving mass behind in an empty Cell still applies for Low Precision runs. This can be addressed by defining a (small) non-zero Lower Bound. Some mass will still be left behind in the Cell, but the error can be minimized by making the Lower bound suitably small.

Although this approach is certainly easy to implement, it comes with a potential cost. The fractional timesteps (used in Medium and High Precision runs) provide significant accuracy improvements (with minimal computational expense) during periods when the media amounts are not changing rapidly. Moreover, other variables controlled by the Solution Precision can play an important role in more complex models (e.g., with different types of mass transport processes, more complex transient behavior, isotopes, solubility constraints, etc.).

So for some models (particularly those with no solubility constraints, no rapidly decaying species and no isotopes) you may indeed be able to simply add a Lower Bound and run at Low Precision to avoid spikes. However, you may then need to decrease the size of the timestep to accurately solve the mass transport equations. For complex mass transport models (e.g., with rapidly decaying species, solubility constraints and/or isotopes), however, using Low Precision is not recommended, and the approach discussed below should be used.

#### Approach 2: Dynamically Adjust Timestep

In this approach, we take advantage of the accuracy improvements of the Medium and High Precision setting (when Cell media amounts are not changing rapidly) while also avoiding the inaccurate behavior (when they are changing rapidly).

The approach to doing so is to reduce the error to an acceptable level by dynamically adjusting the timestep only when these problems occur.

This can be done as follows:

1. Create a non-zero Lower Bound for the media amounts that are rapidly changing in the Cell (typically the Reference Fluid water, but could be another Fluid, or a Solid if you were simulating advection in these media).
2. Define a maximum timestep allowed for that Cell based on the Cell media amount, and the inflows and outflows of that media.

Assuming that the volume of the Cell that we are concerned with is computed using a Pool element (named, for example, **Volume1**), we would define an Expression (e.g., **MaxStep1**) that defines the maximum allowable timestep as follows:

```
if(Abs(Net_Out) > 0 m3/day and Volume1.Total_Outflow* Default_DT /
Volume1>Allowed_Fraction, Allowed_Fraction*Volume1/abs(Net_Out),
Default_DT)
```

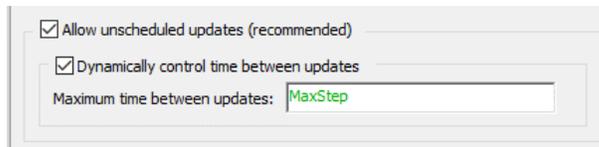
In this equation, **Default\_DT** is the default scheduled timestep and **Net\_Out** is the total outflow rate minus the total inflow rate:

```
Volume1.Total_Outflow-Volume1.Total_Inflow
```

The **Allowed Fraction** is the maximum allowable fractional change that we select to appropriately minimize the error. GoldSim provides a warning message (when running with Medium or High Precision) if the fractional change is greater than 10%. For many systems, the fractional change will likely need to be higher than this to produce a significant error, but the warning is conservatively displayed at 10%.

Experimentation will be required to determine the appropriate value. You want to use the largest value that minimizes the error to an acceptable level (the smaller the value, the higher the computational expense).

3. If there are multiple Cells that may potentially be changing rapidly in this way, repeat step # 2 for each Cell and then compute the minimum of these values.
4. Enter this value into the field defining the **Maximum time between updates** in the **Advanced Time Settings** (accessed via the **Time** tab of the Simulation Settings dialog):



**Note:** Dynamically changing the timestep is discussed in Chapter 7 of the **GoldSim User's Guide**.

This algorithm works very well and is generally very efficient (the timestep is only minimized rarely and when it needs to be).

The two parameters that control the accuracy are the **Allowed Fraction** and the **Lower Bound**. The smaller these values, the smaller the error. Of course, as these values are reduced, the timestep becomes smaller (and the computational effort increases). As a result, some experimentation may be required to determine the most appropriate values for a particular system. As pointed out above, for most systems, the fractional change will likely need to be greater than 10% to 20% or so to produce a significant error. Of course, a larger Lower Bound also results in more mass left behind in an “empty” Cell, but in many cases, this may not pose a problem (e.g., it quickly re-enters the system when the Cell refills).

The higher the net outflow (**Net\_Out** above) as the volume approaches zero, the greater number of timesteps that will be required (e.g., the smaller **Allowed Fraction** may need to be). It should be noted, however, that in the real-world,

outflow rates generally decrease as the volume decreases (due to natural feedback loops). For example, as the volume of a pond decreases, the surface area of the pond decreases, and the evaporation rate decreases. Similarly, as a pond volume decreases, the pumping rate will often be lowered (e.g., either by turning off one of several pumps or adjusting the pumping rate of variable speed pumps). These kinds of feedback loops result in a more gradual approach to the Lower Bound (and it is strongly recommended that you represent them in your model if they are present).

### Managing Excessive Transport Rates

Sometimes you may specify a very high mass transfer rate (either advective, diffusive, or other) in order to "flush out" a Cell element.

The GoldSim solution algorithm cannot accommodate excessively high transport rates. Therefore, GoldSim tests for excessive transport rates in mass flux links, and outputs a warning message if the transport rate for any species exceeds  $10^7$  of the current mass per timestep. If you see such warnings in your Run Log, you should reduce the transport rate to a value which is not so excessive. Failure to do so may result in inaccurate results.

### Saving Results for a Cell

Cell pathways produce the following outputs:

- the total mass of each species in the pathway;
- the concentration of each species in each medium; and
- the mass flux of each species for any specified advective Outflows and diffusive Outfluxes.

Other (optional) outputs include the amount of precipitated mass in the pathway, and the dissolved concentration of species in a fluid that contains suspended solids.

These outputs are all vectors by species. Media concentrations have dimensions of mass/volume for Fluids and mass/mass for Solids. Fluxes have dimensions of mass/time.

You specify that you wish to save these results in three different places:

1. Species masses (and precipitated masses, if **Output Precipitated Mass** is checked) in the pathway are saved by clicking **Final Values** and/or **Time History** at the bottom of the Cell editing dialog.
2. Concentrations are saved by selecting a medium in the media list in the Cell editing dialog and clicking Save Final Concentration (labeled "**F**") and/or Save Concentration History (labeled "**H**") directly to the right of the selected medium:

Media in Cell			
Medium	Amount	F	H
Water	120 m3	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Sediments	60 kg	<input checked="" type="checkbox"/>	<input type="checkbox"/>



**Note:** You cannot check the Save Concentration History box if you are running multiple realizations. As discussed below, in order to save histories when running multiple realizations, you must connect the output of interest to a Time History Result element.

3. Fluxes are saved by selecting a mass flux link in the Inflows, Outflows or Diffusive Fluxes tab for a linked Cell and clicking **Save Final Values** and/or **Save Time History** at the bottom of the dialog:

Properties of Selected Outflow

Outflow: Pond1.Water\_to\_Pond2

Link Type: Coupled

Flow Rate: 10 m3/day

Species flux rates:  Save Final Values  Save Time History

If you are running multiple realizations, the Time History box is ignored, and unless an output of the element is connected to a Time History Result element, no time history results will be saved at all for the element. In fact, in such a case, the Save Results section (for items 1 and 3 above) would look like this:

Final Values  Monte Carlo Histories

In this particular case, because the simulation involves multiple realizations, the “Time History” checkbox is replaced by a “Monte Carlo Histories” checkbox. This checkbox is grayed out, since it is only used for information purposes. You cannot edit it directly, and its appearance is completely determined by whether or not the output is connected to a Time History Result element. That is, in order to save time history results for a Cell output when running multiple realizations, you must connect it to a Time History Result element.

The display units for masses, concentrations and fluxes for all pathways are specified in the **Contaminant Transport** tab of the Options dialog (accessed via **Model | Options...** from the main menu):

Options

General | Graphic | Results | Modules | Contaminant Transport

General Options

Solution precision: Medium (default)

Log warning messages  Disable decay of species

Log cell-network details

Source Term

Barrier failure type: Random failure time

Round (vs truncate) the computed number of waste-package failures

Display Units

Mass in pathways: g (M)

Mass fluxes: g/yr (M/T)

Fluid concentrations: mg/l (M/L3)

Solid concentrations: g/kg (M/M)

Restore defaults

OK Cancel Help

## Using Aquifer Pathways

An Aquifer pathway is intended to represent a feature that essentially behaves as a *fluid conduit*. It provides a way to simulate processes such as vertical transport through an unsaturated (vadose) zone or horizontal transport in aquifers, rivers, channels and pipelines.

Note that a similar pathway, the Pipe, can be used for many of the same purposes. A discussion of the advantages and disadvantages of Pipes and

## Features and Capabilities of Aquifers

Aquifers, and when each should be used, is provided in the referenced section below.

**Read more:** [Comparing Pipes and Aquifers](#) (page 89).

An Aquifer pathway actually performs its computations by creating a temporary set of linked Cell elements during the simulation, which are subsequently removed at the end of the simulation. In most cases, there is no need for you to be aware of how this is done, or to view the temporary Cell pathways that are created.

The geometry of the pathway is defined by specifying an Aquifer Length and an Aquifer Area. You must also define the Number of Cells to be used to discretize the system. Based on this, GoldSim internally creates a series of linked Cell pathways. The specified Infill Medium and Fluid Saturation are used to determine the quantities of media in each Cell. A pathway Dispersivity is also specified. Advective and diffusive flux links are automatically created by GoldSim to appropriately model advection, dispersion and diffusion through the linked Cells.

**Read more:** [Understanding How an Aquifer Pathway Works](#) (page 189).

Mass enters at one end of an Aquifer, advects through (and disperses and diffuses within) the Aquifer, and then exits at the other end. Aquifer pathways (and hence the Cells that are internally created to represent them) contain only a single fluid medium (which is always, by definition, the Reference Fluid), and an optional single solid medium which can impact transport (e.g., by modifying the porosity of the pathway and/or acting to sorb and hence retard species).

Because Aquifers internally use Cells to carry out their calculations, they can represent most of the same processes that can be represented by a Cell network. In particular, Aquifers can represent the following:

- **Partitioning.** Within each internal Cell contaminants are partitioned between the the Reference Fluid and Infill Medium based on the partition coefficients and masses/volumes of the various media present.
- **Solubility constraints.** You can assign solubility limits for the contaminants in the Reference Fluid (typically water) present in the pathway. The dissolved concentrations of the contaminants in the pathway cannot exceed the solubility limits. If you are simulating isotopes of the same element, GoldSim ensures that the sum of the concentrations of all isotopes does not exceed the solubility limit.
- **Mass transport.** Advective, dispersive and diffusive transport mechanisms are explicitly represented within the pathway (using advective and diffusive mass flux links between the internal Cells).
- **Suspended Solids** can be specified to be present in the Aquifer. These Solids are assumed to be advected and dispersed along the Aquifer. Species which partition onto the suspended Solids are transported with them as they move through the Aquifer.

Because the Cells are linked together via advective and diffusive mechanisms, the behavior of the Cell network is mathematically described using a coupled system of differential equations. In effect, the network of Cells created within an Aquifer pathway is mathematically equivalent to a finite difference network. GoldSim numerically solves the coupled system of equations to compute the contaminant mass present in the pathway (and the mass fluxes leaving the pathway) as a function of time.



**Note:** If the Cell network created by an Aquifer pathway is too simple, and you need to represent a more complex Cell network (e.g., two-dimensional and/or homogeneous), and/or you do not want the Cell network to be temporary, you can use a CellNet Generator to automatically and rapidly create Cell networks.

---

**Read more:** [Automatically Generating Cell Networks Using the CellNet Generator](#) (page 151).

The following sections describe the basic assumptions incorporated into Aquifer pathways, and how to define and use them in your models. The mathematical and computational details of how Cell pathways (and hence Aquifer pathways) are implemented within GoldSim are provided in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

## Aquifer Pathway Example: Advection, Retardation and Dispersion

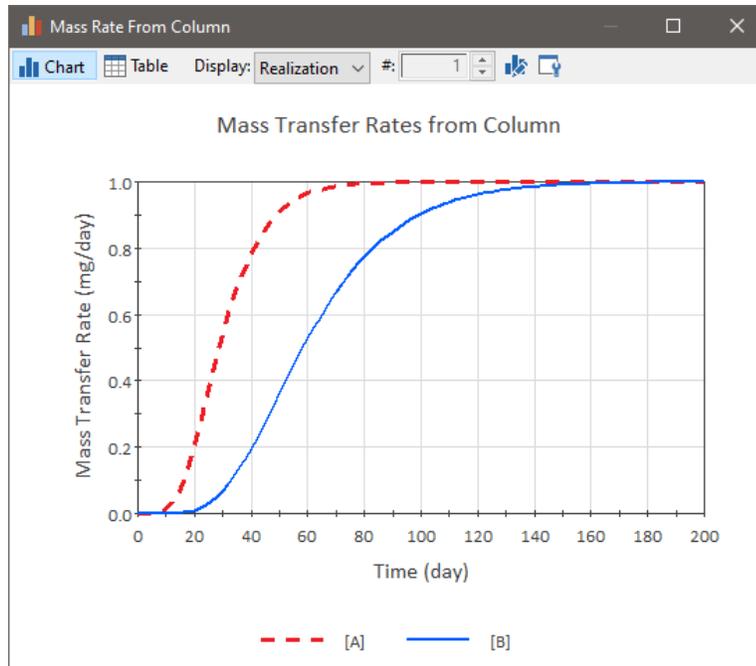
Before describing the details involved in using Aquifer pathways, it is worthwhile to present an example illustrating some of their basic capabilities. This particular example model, Aquifer.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

Suppose that you wish to simulate a simple column experiment. In this experiment, water flows at a constant rate through a saturated cylindrical column filled with sand (porosity of 0.3 and bulk density of  $1600 \text{ kg/m}^3$ ). The column is 2 m long and has a cross-sectional area of  $0.05 \text{ m}^2$ . Water flows through the column at a rate of  $1\text{E-}3 \text{ m}^3/\text{day}$ , and the dispersivity is assumed to be 10% of the column length. At one end of the column, two species (A and B) are injected at a rate of 1 mg/day. A does not partition onto the sand, but B does, with a partition coefficient of  $2\text{E-}4 \text{ m}^3/\text{kg}$ . You wish to simulate the breakthrough of the two species out the end of the column.

To simulate this system in GoldSim, you would do the following:

1. Define two species (A and B);
2. Define two media (Water and Sand) and specify their properties;
3. Define a single Aquifer to represent the column;
4. Specify the properties of the Aquifer;
5. Define a sink Cell and create an advective mass flux link from the Aquifer to the Cell.
6. Specify the (upstream) boundary condition for the Aquifer; and
7. Specify the simulation settings (i.e., duration and timestep) and run the model.

The output of this simulation, in the form of time histories of the mass transfer rate of species A and B exiting the column, is shown below:



The mean unretarded travel time (which can be thought of as the travel time in the absence of dispersion),  $t$ , through an Aquifer can be computed as follows:

$$t = n A L / Q S$$

where  $n$  is the porosity of the infill,  $A$  is the cross-sectional area of the Aquifer,  $L$  is the length of the Aquifer,  $Q$  is the flow rate, and  $S$  is the degree of saturation of the fluid.

In this example,

$$t = (0.3)(0.05 \text{ m}^2)(2 \text{ m}) / 1\text{E-}3 \text{ m}^3/\text{day} = 30 \text{ days}$$

As can be seen from the figure, the unretarded species (A) reaches 50% of its steady state flux rate just prior to 30 days (due to the impact of boundary conditions, the solution to the equation is asymmetric and the 50% breakthrough value is expected to occur slightly before the calculated mean travel time). The spread around this point is due to dispersion in the pathway. Species B reaches 50% of its steady state flux at about 60 days. This is because the effective retardation factor,  $R$ , in this particular case can be computed as:

$$R = 1 + \frac{(\rho_b)(K_d)}{n} = 1 + \frac{(1600 \text{ kg/m}^3)(2\text{E-}4 \text{ m}^3/\text{kg})}{0.3} = 2.1$$

where  $\rho_b$ ,  $K_d$  and  $n$  are the bulk density, partition coefficient and porosity, respectively, for the Solid infill through which the fluid is flowing.

Hence, in this example, the breakthrough curve for B was retarded by about a factor of two.

The editing dialog for an Aquifer pathway is shown below:

## Defining Basic Aquifer Properties

The basic Aquifer properties are listed on the main Aquifer dialog, and are described below.

### Aquifer Geometry

The first two input fields in the Aquifer pathway dialog describe the overall geometry of the pathway.

**Length:** This is the length of the pathway. Note that the length can change dynamically to represent processes such as erosion.

**Area:** This is the total cross-sectional area of the pathway. If an infill medium is specified, it fills the area.



**Note:** If a non-zero **Source Zone Length** is defined, the Aquifer Length and Area must be static (cannot change dynamically).

**Read more:** [Controlling How Mass Enters an Aquifer](#) (page 184).

### Other Basic Aquifer Properties

In addition to the inputs describing Aquifer geometry, Aquifers require four additional inputs that control the basic behavior of the Aquifer:

**Dispersivity:** This is the longitudinal dispersivity of the pathway. It has dimensions of length. The longitudinal dispersivity acts to spread or disperse species around the mean travel time as they are transported through the Aquifer. Different systems disperse solutes to different degrees. A good first approximation for one-dimensional transport through a relatively homogeneous aquifer might be that the dispersivity is 10% of the total length of the pathway. You must specify a dispersivity which is greater than or equal to zero.

**Number of Cells:** This is the number of temporary Cell elements that will be created internally to carry out the calculations. In order to avoid numerical dispersion, the number of Cells should be no less than the Length divided by twice the dispersivity. (If the Number of Cells is too small, GoldSim will write a warning to the Run Log). The maximum number of Cells is 100 (as there would be little benefit in using a number greater than this), and the minimum number of Cells is 4. If you specify a value outside of this range, GoldSim adjusts the number of Cells accordingly and writes a warning message to the Run Log. Note that this value must be constant (it cannot change with time).

**Read more:** [Understanding How an Aquifer Pathway Works](#) (page 189).

**Infill Medium:** This is the (optional) porous medium that fills the (entire) pathway. It must be an existing Solid medium in the model. You can, however, specify that there is no porous medium filling the pathway (e.g., if you were simulating a channel or river) by leaving this field blank.

The porous medium affects the behavior of the Aquifer in two ways: 1) it increases the flow velocity (by reducing the effective flow area); and 2) it can act to retard any species which partition onto it.

**Fluid Saturation:** This is the degree of saturation of the Aquifer. It is dimensionless, and must be greater than 0 and less than or equal to 1. If you were simulating a saturated aquifer or a river, you would specify the fluid saturation as 1 (the default). If, however, you were simulating flow through an unsaturated porous medium (e.g., surface soils or a vadose zone), this would be specified as less than 1.

Decreasing the fluid saturation affects the behavior of the Aquifer in two ways: 1) it increases the flow velocity (by reducing the effective flow area); and 2) it increases the degree of retardation due to partitioning onto the porous infill (by reducing the effective volume of fluid present in the pathway relative to these solids).

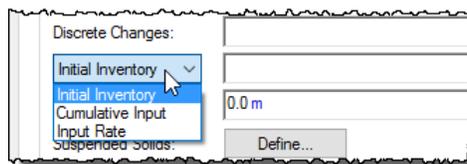
### Defining Initial/Boundary Conditions for an Aquifer

There are two ways by which species mass can enter an Aquifer:

- Through a mass flux link from another pathway to the Aquifer; and/or
- By defining an initial and/or a boundary condition for the Aquifer.

In this section, we discuss defining an initial and/or boundary condition for an Aquifer.

An initial condition/boundary condition for an Aquifer is specified using the drop-list directly below the Discrete Changes field within the Aquifer dialog. This drop-list provides three options:



In all three of these cases, if the **Source Zone Length** is zero (the default), the mass is applied at the beginning of the Aquifer (the first Cell). If the **Source Zone Length** is greater than zero, the mass is distributed uniformly over the specified length.

**Read more:** [Controlling How Mass Enters an Aquifer](#) (page 184).

- **Initial Inventory.** This is the default, and represents the initial inventory of each species in the pathway. This field only accepts vectors by species with dimensions of mass. Moreover, this input cannot be specified as a function of time (if it is, GoldSim will display a fatal error when you try to run the model).
- **Cumulative Input.** This option provides a mechanism for simultaneously specifying an initial condition *and* a rate of mass addition (that may change with time). This field only accepts vectors by species with dimensions of mass. It represents the *cumulative* amount of mass of each species added to the Aquifer at a given time. Hence, if it is constant, it represents an initial condition. If it increases with time, its rate of change represents a specified rate of addition. Correct use of the "Cumulative Input" is summarized in the table below:

To specify this:	Enter the following into the "Cumulative Input" field:
An initial condition (at the beginning of the Aquifer)	A constant vector with dimensions of mass
An initial condition and a <i>constant</i> rate of addition (at the beginning of the Aquifer)	An expression such as: $Initial + Rate * Etime$ , where Initial is a constant vector (with dimensions of mass) and Rate is a constant vector (with dimensions of mass/time).
An initial condition and a <i>time-variable</i> rate of addition (at the beginning of the Aquifer)	The output of a Pool, Reservoir or Integrator element (with output dimensions of mass) with a specified Initial Value and (time-variable) Rate of Change.



**Warning:** The Cumulative Input must stay constant or increase with elapsed time. That is, you cannot remove mass from an Aquifer using the Cumulative Input field. If the value ever begins to decrease with time, a fatal error occurs.

- **Input Rate.** The third option is used to specify a rate of mass addition (that may change with time). This field only accepts vectors by species with dimensions of mass/time. It represents the rate at which mass of each species is added to the Aquifer over the next timestep.



**Note:** One way to easily enter a vector of data into an input field without having to create a separate element is to use GoldSim's vector constructor function. For example, entering "vector(1g)" into the Cumulative Input field results in an initial condition of 1 g of each species being present in the Aquifer.

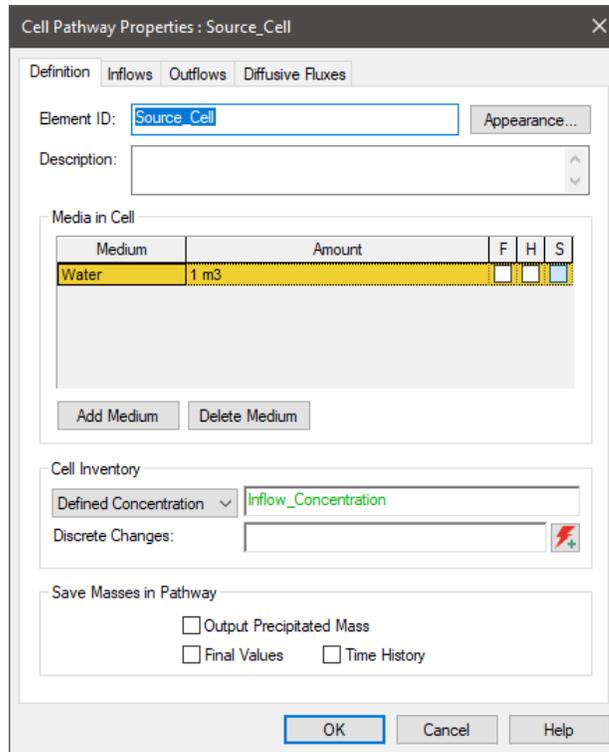
Although the **Input Rate** and **Cumulative Input** options provide a quick and convenient way to enter mass input rates, if mass input rates into an Aquifer are changing with time (e.g., because the inflow concentration is changing), a slightly more accurate way (both numerically and conceptually) to specify such a boundary condition is to create a “Source Cell” that is defined using a **Defined Concentration**.

**Read more:** [Defining Initial and/or Boundary Conditions for a Cell](#) (page 126).

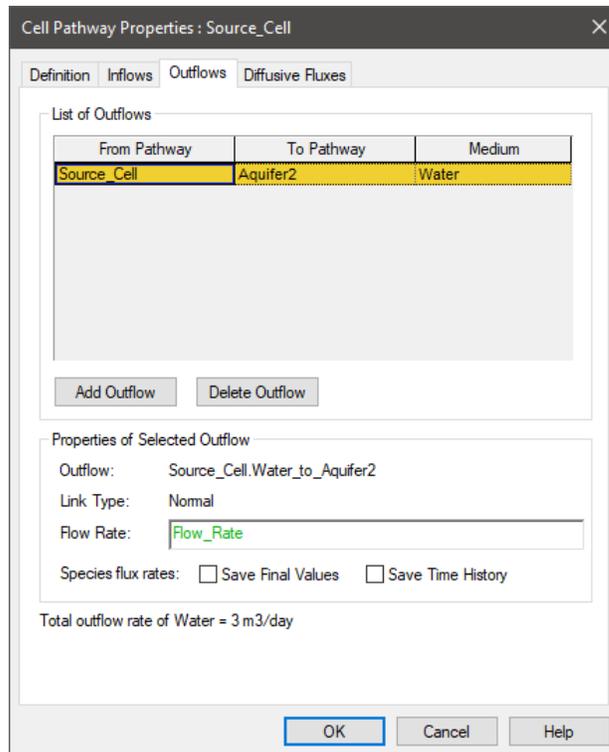
As an example, consider a case in which you have a boundary condition with a constant inflow rate (Flow\_Rate) and a time-varying Inflow\_Concentration. The Aquifer has a constant outflow rate (equal to the inflow rate). You could model this in two ways:

- In the first approach, you simply provide an **Input Rate** to the Aquifer:

- In the second approach, you define a “Source\_Cell” that looks like this:

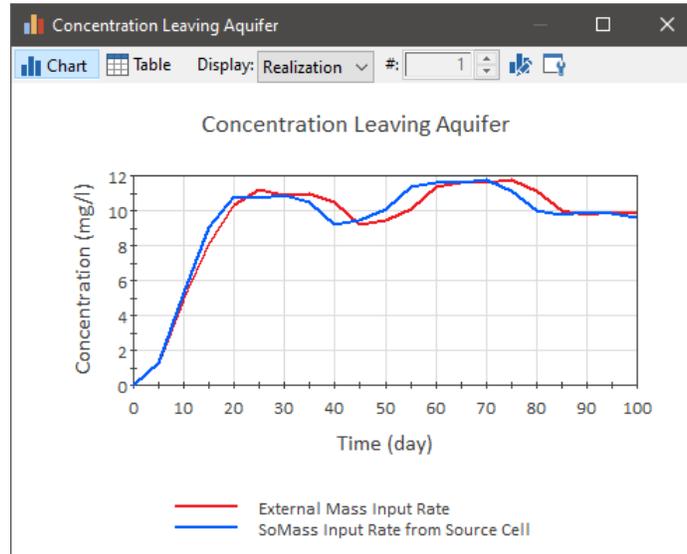


The volume is set to an arbitrarily small number (it is not used to compute concentrations since the concentration is fixed). A **Defined Concentration** is specified for this Source\_Cell that will flow into Aquifer. That is, the Source\_Cell has an outflow to the Aquifer:



The Aquifer itself has no **Input Rate** specified.

If we run this model (for 100 days with a 5 day timestep) and compare the results for these two different approaches to representing the boundary condition (in terms of the concentration leaving the Aquifer), they look like this:



What we see is that the mass that is input “externally” (using the **Input Rate**) lags by one timestep. This is because in this, due to the way the external boundary condition must be applied when solving the pathway equations, a one timestep lag is introduced. Hence, the second approach is a more accurate representation (although for a small timestep, the differences would likely be insignificant). Conceptually, however, this is a bit more accurate way to represent the boundary condition (since the boundary condition is actually treated as part of the pathway network).

In addition to specifying the input boundary condition for an Aquifer, you can also control the output boundary condition. In particular, the checkbox **Enable dispersive and diffusive outfluxes to downstream pathway(s)** changes the outflux boundary condition.

If this box is cleared (the default), only advective transport out of the pathway is allowed. If the box is checked, a zero concentration in the receiving pathway is assumed, and dispersive and diffusive transport into downstream pathways is allowed.

These two boundary condition options represent two possible extremes for the behavior of the system. The actual behavior of most real-world systems would be somewhere between these two extremes (although in most real-world systems, it will be very close to either one or the other). The default boundary condition (no dispersive and diffusive fluxes) is most appropriate if the downstream concentration is similar to the concentration leaving the pathway. In this case, the concentration gradient is small (and hence the dispersive and diffusive fluxes would be small). If the box is checked, dispersive and diffusive transport into downstream pathways is allowed (assuming a zero concentration in those pathways). This might be appropriate, for example, if the downstream pathway represents a rapidly-flowing, “clean” pathway.

The impact of this boundary condition can be evaluated by comparing the behavior of an Aquifer to the behavior of the same system simulated using a different solution technique and boundary condition (the Pipe pathway, which uses a Laplace transform solution).

### Simulating Discrete Changes to the Mass Inventory in an Aquifer

**Read more:** [Comparison of Aquifers and Pipes for Simulating a One-Dimensional Pathway](#) (page 251).

In addition to adding mass to an Aquifer via an initial/boundary condition, and adding/removing mass via mass flux links, GoldSim allows you to instantaneously add species mass to an Aquifer.

This is done using the **Discrete Changes** field in the Aquifer dialog:



This field only accepts discrete change signals. (Discrete change signals are discussed in detail in "Simulating Discrete Events" in the **GoldSim User's Guide**.) The discrete change signal must be a vector by species and have dimensions of mass. Typically, such a discrete change signal will be the output of a Discrete Change element that has been triggered by an event.

Discrete change signals have an *instruction* associated with them. Two types of instructions are possible: Add and Replace. The Discrete Changes field for an Aquifer only accepts Add signals.

When an Add signal is sent to an Aquifer during a simulation, the specified amount of mass of each species in the discrete change vector is added to the first Cell in the network representing the pathway.



**Note:** The discrete change vector cannot contain negative numbers (i.e., you can NOT discretely remove mass from an Aquifer; you can only add mass).

Like most input fields that accept discrete change signals, you can specify multiple discrete changes. You can do this in two ways:

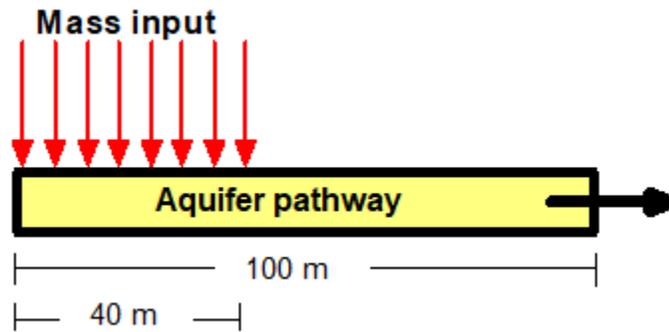
1. You can enter multiple discrete changes into the input field by separating the entries using a semi-colon; and
2. You can use the Multiple Discrete Changes button to the right of the input field (i.e., the small button with two exclamation marks) to access a table listing the Discrete Changes (to which you can add or delete entries).

In the latter case, any Discrete Changes which are added to the list are also automatically added to the input field, separated by semi-colons.

The Discrete Changes field can be very useful for instantaneously modifying your system in response to discrete events. Note, however, that this feature should be used with care, since when it is applied, conservation of mass in the system is the responsibility of the user.

### Controlling How Mass Enters an Aquifer

GoldSim allows you to control where mass enters an Aquifer by specifying a **Source Zone Length**. This represents a length along the flow direction in the pathway. Hence, if your pathway had a length of 100m, and you specified a **Source Zone Length** of 40m, mass would enter the pathway uniformly over the first 40m (rather than at the beginning of the pathway):



This is useful, for example, if your Aquifer represents an aquifer which is being loaded from above with mass from source which is of such an areal extent (e.g., a landfill) that it extends over a significant portion of the pathway and therefore cannot be treated as a point source.

By default, the **Source Zone Length** for an Aquifer is zero. In this case, any mass entering the Aquifer is treated as a point source which is applied at the beginning of the Aquifer (the first Cell). If the **Source Zone Length** for an Aquifer is greater than zero, the mass is distributed uniformly over the specified length.

A number of points regarding the use of the **Source Zone Length** are worth noting:

- The **Source Zone Length** must be static (it cannot change with time).
- If a non-zero **Source Zone Length** is defined, the Aquifer Length and Area cannot change with time (doing so would generate a fatal error).
- The **Source Zone Length** is applied to all forms of mass that enter the Aquifer: mass that enters as an initial or boundary condition, mass that enters the Aquifer from other pathways via a mass flux link, and mass that enters the Aquifer as a specified discrete change via the **Discrete Changes** field.
- If the **Source Zone Length** is larger than the Aquifer **Length**, the **Source Zone Length** is assumed to be equal to the Aquifer Length (and a warning message is written to the Run Log).



**Warning:** The Source Zone Length should only be used if the total flow in the Aquifer is substantially larger than the flow associated with the incoming mass. This is because that the Source Zone Length does not change the flow rate along the Aquifer (all of the pathway's inflows are assumed to enter at the beginning of the pathway); it only impacts where the mass is input. Hence, it is equivalent to assuming that the amount of flow associated with the mass entering the pathway is negligible relative to the total flow in the pathway (e.g., associated with "clean" upgradient water).

## Simulating Suspended Solids in an Aquifer

GoldSim allows you to specify that suspended Solids are present in the Aquifer. These Solids are assumed to be advected and dispersed along the Aquifer. Species which partition onto the suspended Solids are transported with them as they move through the Pipe.

Suspended solids are specified to be present in the Aquifer via the **Suspended Solids...** button on the Aquifer dialog. When you press this button, the following dialog is displayed:

An Aquifer can have a single suspended Solid for which you must define the **Solid Medium** and the **Concentration**:

**Solid Medium:** This is the solid suspended in the Aquifer. It must be a previously defined Solid medium.

**Concentration:** This is the concentration of the suspended solid in the Aquifer fluid. It has dimensions of mass per volume.

Suspended solids in an Aquifer can increase the "carrying capacity" of the pathway fluid, by allowing solute species to sorb onto and be transported by particulates. This has the effect of reducing retardation due to sorption onto infill material. Mathematically, suspended solids in an Aquifer can be thought of as increasing the effective concentration in the pathway fluid, thereby increasing the mass flux of species out of the Aquifer. In particular, assuming no dispersion, the advective mass flux of species  $i$  leaving the Aquifer,  $\text{Flux}_i$ , becomes:

$$\text{Flux}_i = Q \text{cd}_i (1 + K_i V_{\text{susp}} c_{\text{susp}})$$

where  $Q$  is the flow rate in the Aquifer (volume/time),  $\text{cd}_i$  is the dissolved concentration of species  $i$  (mass/volume),  $K_i$  is the partition coefficient for species  $i$  for the suspended solid medium (volume/mass),  $c_{\text{susp}}$  is the suspended solid concentration (mass/volume), and  $V_{\text{susp}}$  is the dimensionless Advective Velocity Multiplier for the suspended Solid (a property of the Solid).

**Read more:** [Advanced Solid Properties](#) (page 77).



**Note:** The suspended solid concentration only impacts advective mass flux links leaving the Aquifer and does not have any impact on the diffusion of particulates into the Aquifer. That is, if a diffusive mass flux link is created between a Cell containing a suspended solid and an Aquifer containing the same suspended solid, for the purpose of simulating the diffusive flux of particulates, the concentration of particulates on the Aquifer side of the link is assumed to be zero.

**Read more:** [Flux Links to/from Aquifers](#) (page 188).

## Aquifer Pathway Outputs

Aquifer pathways have at least two outputs:

- **Mass\_in\_Pathway.** This is a vector by species with dimensions of mass. It represents the total mass of each species in the Aquifer (the sum of the mass in each Cell of the network).
- **Concentration.** This is a vector by species with dimensions of mass per volume. It represents the concentration of each species in the Reference Fluid at the point where it exits the Aquifer (i.e., the *last* Cell).

in the network). This is a “total concentration”, and includes species sorbed onto suspended solids.

In addition, for every advective mass flux link in which the Aquifer is the Outflow (upstream) pathway, an output is created on the Aquifer:

- **Medium\_to\_Path2**, where *Medium* is the name of the flowing medium, and *Path2* is the name of the linked (Inflow) pathway. This is a vector by species, and has dimensions of mass/time. It represents the mass flux of each species from the Aquifer to the downstream pathway.

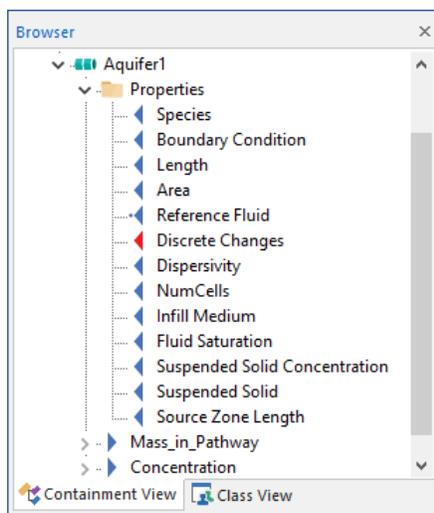
**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94).

It is important to understand that the mass flux outputs from an Aquifer represent the mass rate over the *previous* timestep. This can have implications if you choose to integrate one of these outputs (using an Integrator).

**Read more:** [Manipulating Pathway Outputs](#) (page 253)

## Viewing an Aquifer in the Browser

The browser view of an Aquifer pathway is shown below:



The *Properties* folder contains all the inputs for the Aquifer. The *Inflows* and *Outflows* folders contain all of the mass flux links for the Aquifer.



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

The pathway's mass and concentration outputs are listed first. Note that for an Aquifer, the concentration always refers to that in the Reference Fluid.

The *Properties* folder contains the basic inputs for the Aquifer. With two exceptions (listed below), you can create a link to any of these property inputs using the Link Cursor.

Note that the *Species* input and the *Reference Fluid* input also appear in the *Properties* folder. The *Species* input is automatically linked to the nearest *Species* element when the Aquifer is created. Similarly, the *Reference Fluid* input is automatically linked to the nearest *Reference Fluid* element when the

### Flux Links to/from Aquifers

Aquifer is created. *These links cannot be changed using the Link Cursor, and are displayed for information purposes only.*

If the Aquifer has any mass flux links associated with it, the corresponding inputs and outputs for these links are organized into the Inflows, Outflows, and Diffusive Influxes folders. These folders are not shown if they are empty.

**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94); [Inputs and Outputs Associated with Diffusive Mass Flux Links](#) (page 101); [Inputs and Outputs Associated with Direct Transfer Mass Flux Links](#) (page 105); [Inputs and Outputs Associated with Precipitate Removal Mass Flux Links](#) (page 110); [Inputs and Outputs Associated with Treatment Mass Flux Links](#) (page 116).

The only way to transport mass *out* of an Aquifer is by specifying an advective mass flux link to another pathway. Diffusive mass flux links (diffusive outfluxes), and special purpose mass flux links (direct transfer, precipitate removal and treatment) *from* Aquifers cannot be created.

**Read more:** [Understanding Advective Mass Flux Links](#) (page 90).

Advective mass flux links are used to transport mass via a flowing medium. Mass which is dissolved, or suspended within the flowing medium is transported with the medium as it moves. For Aquifer pathways, the flowing medium is always the Reference Fluid.



**Note:** If you specify that the flow rate leaving an Aquifer changes suddenly with time, it will change instantaneously throughout the pathway. Although such a response may be appropriate for a confined aquifer system, for a phreatic system, flow changes would not physically propagate instantaneously (the response would be much slower and would propagate as a “wave”). As a result, when changing the flow rate (for a phreatic system) you should be aware of how it will be represented in GoldSim (and generally should only change it slowly). Of course, in most realistic situations, unless you are applying an artificial sudden change (e.g., pumping), flow rates will in fact change slowly (not suddenly).

---

You can transport mass *into* an Aquifer via an advective mass flux link from any other type of pathway and/or via a diffusive mass flux link from a Cell pathway. Within GoldSim, the concentration and diffusive length on the Aquifer side of a diffusive mass flux link are assumed to be zero. Hence, like advective mass flux links, diffusive mass flux links involving Aquifers are uni-directional.



**Warning:** GoldSim does not enforce a balance for the flow of the Reference Fluid in an Aquifer. That is, the Inflows into an Aquifer do not need to be equal to the Outflows from the Aquifer. If the specified Outflows are greater than the specified Inflows, conceptually the effect on the species concentrations leaving the Aquifer is one of dilution, since "clean" fluid is assumed to be flowing into the Aquifer. If, however, the specified Outflows are less than the specified Inflows, in the absence of decay and dispersion, the species concentrations leaving the Aquifer would be greater than those entering the Aquifer. Conceptually, GoldSim would assume that a quantity of "clean" fluid (carrying no species mass) flowed out of the Aquifer in order to conserve the flow rate and volume in the Aquifer. Although there are some physical situations in which you may actually want to do this (e.g., in order to simulate the evaporation of Water from an Aquifer), typically such behavior would not be intended. As a result, whenever the Inflows to an Aquifer exceed the Outflows, GoldSim provides a (non-fatal) warning message to the Run Log.

**Read more:** [Mass Balance of Transport Media in Pathway Networks](#) (page 253).

### **Advection and Diffusion of Particulates to/from Aquifers**

Suspended solids can advect and diffuse into and out of Aquifers.

Suspended solids can advect into an Aquifer from another pathway containing suspended solids. Suspended solids can also diffuse into an Aquifer from a Cell or Aquifer containing suspended solids. The species mass associated with the suspended solids in the upstream (Outflow or Outflux) pathway enter the Aquifer regardless of whether suspended solids are specified as being present in the Aquifer. When suspended solids (carrying species mass) enter an Aquifer from another pathway, conceptually, the particulates are assumed to immediately disintegrate upon entering the Aquifer (releasing their species mass to the fluid in the Aquifer). If suspended solids are present in the Aquifer, the species mass will then partition onto these solids.

Particulates can diffuse out of an Aquifer to a downstream pathway if (and only if) the **Enable dispersive and diffusive outfluxes to downstream pathway(s)** box is checked. In this case, the suspended Solid concentration in the Influx pathway is assumed to be zero when computing the diffusive gradient (and, hence, the diffusive flux becomes uni-directional).

When mass associated with particulates leave an Aquifer, the Solid does not have to be specified as being present in the Influx pathway. Conceptually, the particulates are assumed to immediately disintegrate upon entering the Influx pathway, with the species mass which was associated with them instantaneously partitioning among the available media in the pathway.

**Read more:** [Advection of Particulates to/from Cells](#) (page 138); [Diffusion of Particulates to/from Cells](#) (page 141).

### **Understanding How an Aquifer Pathway Works**

An Aquifer pathway actually performs its computations by creating a temporary set of linked Cell elements during the simulation (while in Run Mode), which are subsequently removed at the end of the simulation. However, while in Run Mode, the pathways exist (and if you pause the model, can actually be viewed).

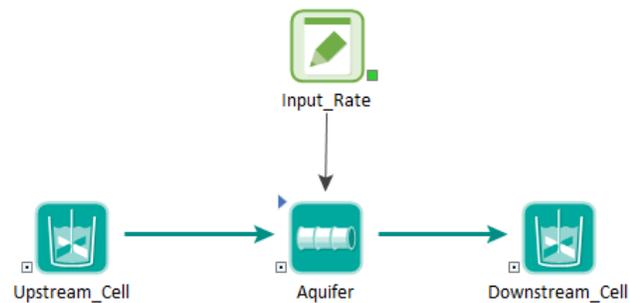
(Pausing a model is discussed in detail in Chapter 7 of the **GoldSim User's Guide**.)

In most cases, there is no need for you to be aware of how this is done, or to view the temporary Cell pathways that are created. For those that are interested, however, this section discusses these operations in more detail.

To illustrate this, and to explain how the various inputs for an Aquifer are mapped onto and treated within the temporary Cell network, we will consider a simple example. In this example, an Aquifer has been defined. Its key properties are as follows:

- The Number of Cells used to discretize the pathway is equal to five.
- The Aquifer contains an Infill Medium (Sand).
- The Aquifer has a single outflow (Q) to a downstream Cell.

While in Run Mode, an Aquifer pathway takes on some characteristics of a Container so that the temporary Cells can be viewed. In this example, if we pause the model during the simulation, the Aquifer pathway will look like this (i.e., like a Container, it has a small triangle in the upper left-hand corner of the element indicating that you can “look inside”):



If we click on the triangle to “look inside” the Aquifer, we see the following:



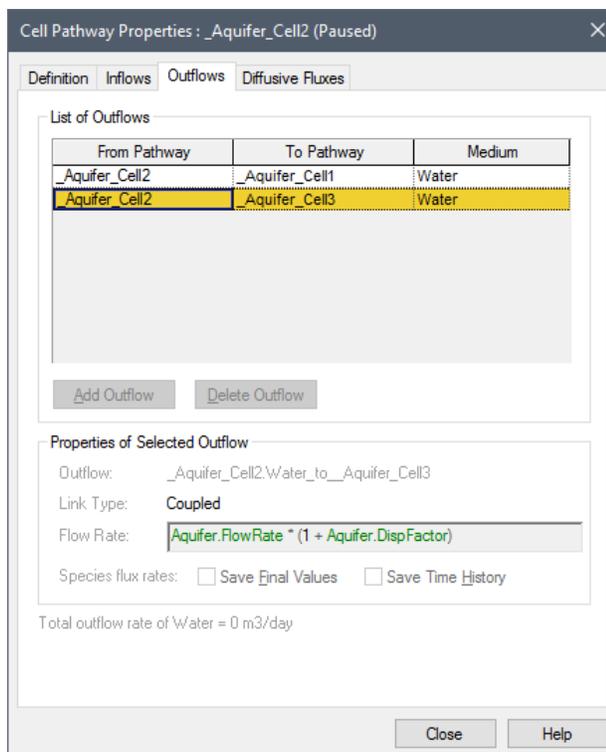
As can be seen, five temporary Cells have been created (named “\_pathwayname\_Celln”). Opening the first Cell, we can see how the Media are defined:

Media in Cell				
Medium	Amount	F	H	S
Water	$Aquifer.OtherCell.Length * Aquifer.Area * Sa$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Sand	$Aquifer.OtherCell.Length * Aquifer.Area * Sa$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

The media quantities are automatically computed based on the Aquifer properties (e.g., Length, Area, Saturation, Number of Cells) and media properties (density, porosity).

In effect, GoldSim has discretized the system into these five finite volumes.

To simulate advection and dispersion/diffusion through the linked Cells, GoldSim automatically creates a number of advective and diffusive flux links. For example, here is the Outflows tab from the second Cell:



There is an Outflow from Cell2 to Cell3. Note, however, that the Flow Rate that was specified when defining the element has been adjusted. The Flow Rate (downstream) from Cell2 to Cell3 is now defined as  $Q*(1+DispFactor)$ , where

$$DispFactor = (n \alpha / L) - 0.5$$

In this equation,  $\alpha$  is the species dispersivity (dimensions of L), L is the pathway length (dimensions of L), and n is the number of cells.

Note that there is another Outflow in the Outflows tab, and it is from Cell2 to Cell1 (upstream!). If we were to look at this, we would see that this upstream Flow Rate was defined as  $Q*DispFactor$ . That is, in addition to the downstream flow that we would expect (Q), GoldSim has added two “fictitious” flows equal to  $Q*DispFactor$  (one upstream and one downstream). Note that since one fictitious flow is downgradient and one is upgradient, the net of these two flows is zero. However, they have the effect of representing longitudinal dispersion in the pathway.

In effect, what GoldSim is doing is using the Cells (the finite volumes) to solve the governing equation describing one-dimensional advective/dispersive transport. We can solve this equation numerically using finite differences. When we do so, we find that the rate of change of mass in, for example, Cell2, accounting for both advection and dispersion, can be approximated as follows:

$$\begin{aligned} \text{Mass Rate of Change in Cell2} = & - Q*C2*(1 + 2*DispFactor) \\ & + Q*C1*(1 + DispFactor) \\ & + Q*C3*DispFactor \end{aligned}$$

where:

Q is the specified flow rate in the Aquifer;

C1 is the concentration in Cell1;

C2 is the concentration in Cell2; and

C3 is the concentration in Cell3.

The derivation of this finite difference approximation is discussed in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

We can now see what the various Outflows that GoldSim automatically created represent. The first term represents the mass flows leaving Cell2. This consists of the advective flow downstream to Cell3 (equal to  $Q \cdot C2$ ) and two dispersive flows (equal to  $Q \cdot C2 \cdot \text{DispFactor}$ ), one upstream to Cell2 and one downstream to Cell3.

The second term is the mass flow entering Cell2 from Cell1 (an advective flow equal to  $Q \cdot C1$  and a dispersive flow equal to  $Q \cdot C1 \cdot \text{DispFactor}$ ).

The third term is the mass flow entering Cell2 from Cell3 (a dispersive flow equal to  $Q \cdot C3 \cdot \text{DispFactor}$ ).



**Note:** Even in the absence of the dispersive terms, a network of linked Cells simulating advective transport will inevitably exhibit a degree of **numerical dispersion** that is a function of the number of Cells (the degree of discretization). In particular, the equivalent numerical dispersivity is equal to  $L/2n$ . As a result, if the number of Cells is less than the pathway length divided by twice the dispersivity, that is,  $n < L/(2\alpha)$ , then the numerical dispersivity will exceed the specified dispersivity. If this occurs, GoldSim records a warning in the Run Log (indicating that you either need to use more Cells or increase the dispersivity to accurately model longitudinal dispersion along the pathway).

---

GoldSim also automatically adds diffusive connections between the Cells to account for diffusion through the pathway (which in most cases is likely to be negligible).

Several other details should also be noted regarding how the temporary Cells are defined:

- All mass input to the Aquifer pathway (advective inflows, diffusive influxes, boundary conditions and discrete changes) are “lumped” together and treated as a Cumulative Input to the first Cell. The one exception to this rule is if a non-zero Source Term Length is specified. In this case, the mass is spread uniformly over the Cells representing the Source Term.
- By default, the temporary Cells are all of the same size. However, if a non-zero Source Term Length is defined, the size of the Cells are adjusted so that the Source Zone is accurately represented. In particular, the boundary of the Cell closest to the edge of the Zone is moved, and then all of the Source Cells upstream of the boundary are adjusted and assigned equal sizes. The remainder of the pathway (downstream of the Source Zone) is then divided equally among the remaining Cells.

**Read more:** [Controlling How Mass Enters an Aquifer](#) (page 184).

- The user controls whether in addition to the advective outflux there is a dispersive/diffusive component of mass transport from the Aquifer to the receiving pathway(s), via the checkbox **Enable dispersive and diffusive outfluxes to downstream pathway(s)** on the element’s

property page. The default behavior does not include such fluxes (the check box is cleared), and only allows for advective transport out of the pathway. Note, however, that it does include diffusion and dispersion (if specified) along the length of the pathway. If the dispersive/diffusive discharge component is enabled it assumes a concentration of zero in the receiving pathway, which is generally a good approximation only if the pathway represents a rapidly-flowing “clean” aquifer or surface water pathway. Note that this mechanism can increase the outflux rate significantly for diffusively-dominated systems.

- If the pathway length changes by more than a small amount (one part in one thousand) during a simulation (e.g., due to erosion) then the existing Cell elements are modified to reflect the new geometry, and the distribution of contaminant masses is mapped onto the new geometry. This approach works for either shortening or lengthening of the pathway. When the pathway is shortened, the mass that was present in the truncated portion of the pathway is treated as part of the outflux for the corresponding time step.



**Note:** When the pathway’s length changes, there may be some irregularities in the outflux rates due to mapping of the prior spatial distribution of species masses onto the new Cell geometry. In general, users should use a larger number of Cells when modeling varying-length Aquifer pathways.

Once the model enters Result Mode, the temporary Cells are removed and can no longer be viewed.

When viewing the results of an Aquifer, the Mass in Pathway output represents the total mass in the pathway (the sum of the masses in all temporary Cells); the Concentration output represents the concentration in the Reference Fluid in the final temporary Cell. If a suspended solid is present, the concentration represents the total concentration (including the load on suspended solids).

## Saving Results for an Aquifer

Aquifer pathways produce the following outputs:

- the total mass of each species in the pathway;
- the concentration of each species in the Reference Fluid exiting the pathway; and
- the mass flux of each species for any specified advective Outflows.

These outputs are all vectors by species. Reference Fluid concentrations have dimensions of mass/volume. Fluxes have dimensions of mass/time.

You specify that you wish to save these results in two different places:

1. Species masses in the pathway and concentrations in the Reference Fluid exiting the pathway are saved by clicking **Final Values** and/or **Time History** at the bottom of the Aquifer editing dialog:

Save Masses and Outflow Concentrations in Pathway			
Masses:	<input checked="" type="checkbox"/> Final Values	<input checked="" type="checkbox"/> Time History	
Concentrations:	<input checked="" type="checkbox"/> Final Values	<input checked="" type="checkbox"/> Time History	

2. Fluxes are saved by selecting a mass flux link in the Inflows or Outflows tab for a linked pathway and clicking **Save Final Values** and/or **Save Time History** at the bottom of the dialog:

Properties of Selected Outflow

Outflow: Aquifer:Water\_to\_Downstream\_Cell

Link Type: Normal

Flow Rate: 1 m3/day

Species flux rates:  Save Final Values  Save Time History

If you are running multiple realizations, the Time History box is ignored, and unless an output of the element is connected to a Time History Result element, no time history results will be saved at all for the element. In fact, in such a case, the Save Results section would look like this:

Final Values  Monte Carlo Histories

In this particular case, because the simulation involves multiple realizations, the “Time History” checkbox is replaced by a “Monte Carlo Histories” checkbox. This checkbox is grayed out, since it is only used for information purposes. You cannot edit it directly, and its appearance is completely determined by whether or not the output is connected to a Time History Result element. That is, in order to save time history results for an Aquifer output when running multiple realizations, you must connect it to a Time History Result element.

The display units for masses, concentrations and fluxes for all pathways are specified in the **Contaminant Transport** tab of the Options dialog (accessed via **Model | Options...** from the main menu):

Options

General Graphic Results Modules Contaminant Transport

General Options

Solution precision: Medium (default)

Log warning messages  Disable decay of species

Log cell-network details

Source Term

Barrier failure type: Random failure time

Round (vs truncate) the computed number of waste-package failures

Display Units

Mass in pathways: g (M)

Mass fluxes: g/yr (M/T)

Fluid concentrations: mg/l (M/L3)

Solid concentrations: g/kg (M/M)

Restore defaults

OK Cancel Help

## Using Pipe Pathways

A Pipe pathway is intended to represent a feature that essentially behaves as a *fluid conduit*. It provides a computationally efficient and accurate way to simulate processes such as vertical transport through an unsaturated (vadose) zone, horizontal transport in aquifers, rivers, channels and pipelines, and in particular, transport through fractured rock masses.

Note that a similar pathway, the Aquifer, can be used for many of the same purposes. A discussion of the advantages and disadvantages of Pipes and

## Features and Capabilities of Pipes

Aquifers, and when each should be used, is provided in the referenced section below.

**Read more:** [Comparing Pipes and Aquifers](#) (page 89).

Pipe Pathways use a Laplace transform approach to provide analytical solutions to a broad range of advectively-dominated transport processes involving one-dimensional advection, longitudinal dispersion (and diffusion), retardation, decay and ingrowth, and exchanges with immobile storage zones (e.g., matrix diffusion).

The geometry of the pathway is defined by specifying a length, a cross-sectional area, and a perimeter. Mass enters at one end of a Pipe (or along some specified length of the pipe), advects through (and disperses and diffuses within) the *mobile zone* of the Pipe, and then exits at the other end. Unlike Cell pathways, Pipe pathways contain only a single fluid medium (which is always, by definition, the Reference Fluid). They can, however, contain solid media which can impact transport (e.g., by modifying the porosity of the pathway and/or acting to sorb and hence retard species).

The boundary condition for the Pipe is as follows:

Concentration goes to 0 as  $x$  goes to  $\infty$ .

Effectively, this allows dispersive/diffusive outfluxes, with a downstream concentration (immediately after the Pipe) that is actually quite close to the concentration in the Pipe (resulting in a low dispersive outflux).

Two types of simple contaminant *retardation processes* can be represented within a Pipe pathway:

- equilibrium partitioning between the fluid in the pathway and a user-specified *infill medium*; and
- equilibrium partitioning between the fluid in the pathway and a user-specified *coating medium* (around the perimeter of the pathway).

In addition to these linear retardation mechanisms, Pipe Pathways can also represent interchanges with two types of immobile *storage zones* along the length of the pathway:

- **matrix diffusion zones**, in which the transfer rate into and out of the zone is proportional to the concentration gradient and the diffusive properties of the zone; and
- a “**stagnant**” **dispersive zone**, in which the transfer rate into and out of the zone is proportional to the concentration difference and the flow rate in the pathway.

Finally, suspended Solids can be specified to be present in the Pipe. These Solids are assumed to be advected and dispersed along the Pipe, but are not subject to retardation processes or interactions with storage zones. Species which partition onto the suspended Solids are transported with them as they move through the Pipe.



**Warning:** Solubility constraints are not applied within Pipes. (They are only applied within Cells and Aquifers). Hence, if the concentration of a species entering a Pipe (e.g., via a boundary condition) exceeds the solubility limit, the concentration leaving a Pipe could exceed the limit.

---

## Advective-Dispersive Transport in Pipes

The following sections describe the basic assumptions incorporated into Pipe pathways, and how to define and use them in your models. The mathematical and computational details of how Pipe pathways are implemented within GoldSim are provided in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

The simplest application of a Pipe pathway is to use it to simulate one-dimensional advective-dispersive transport.

The first step in defining a Pipe pathway is to specify its geometry. The geometry of a Pipe is defined by specifying a length, a cross-sectional area, and a perimeter.

You then specify the flow rate of the Reference Fluid in the pathway (by defining one or more advective mass flux links from the pathway) and a dispersivity. The velocity in the pathway is computed as a function of the flow rate, the cross-sectional area, a user-specified saturation level, and the porosity of the porous medium (if any) which is specified to fill the pathway.

GoldSim then solves the one-dimensional advection-dispersion equation analytically to compute flux rates exiting the pathway. Pipes explicitly represent the decay of species as they flow through the pathway, as well as the ingrowth of daughter products from parent species. Parents and daughters can have completely different transport properties which will be explicitly represented within the pathway.

Two types of linear retardation processes can be represented within a Pipe:

- equilibrium partitioning between the fluid in the pathway and an infill material; and
- equilibrium partitioning between the fluid in the pathway and a coating material (around the perimeter of the pathway).

If you wish to simulate retardation due to partitioning onto an infill material, you must specify a porous Solid medium to represent the infill. Similarly, if you wish to simulate retardation due to partitioning onto a coating material, you must specify a Solid medium to represent the coating (which can be different from the infill medium), and a coating thickness. Fluid within the pore volume of the coating material is assumed to be immobile.

The mobile fluid in the pore volume of the pathway, the immobile fluid within the coating material, the infill material and the coating material are all assumed to be at equilibrium at all times. The effective retardation factor is therefore computed as a function of the properties of the infill and coating media (bulk densities, porosities, and partition coefficients) and the geometry of the pathway (saturation level, cross-sectional area and perimeter).

### ***Pipe Pathway Example #1: Advection, Retardation and Dispersion***

Before describing the details involved in using Pipe pathways, it is worthwhile to present an example illustrating some of their basic capabilities. This particular example file, Pipe1.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

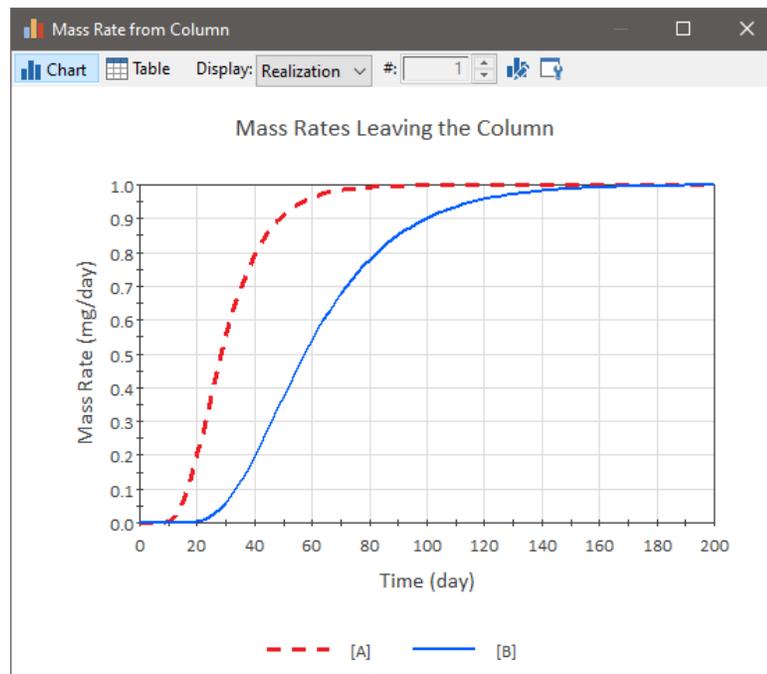
Suppose that you wish to simulate a simple column experiment. In this experiment, water flows at a constant rate through a saturated cylindrical column filled with sand (porosity of 0.3 and bulk density of  $1600 \text{ kg/m}^3$ ). The column is 2 m long and has a cross-sectional area of  $0.05 \text{ m}^2$ . Water flows through the column at a rate of  $1\text{E-}3 \text{ m}^3/\text{day}$ , and the dispersivity is assumed to be 10% of the column length. At one end of the column, two species (A and B) are injected at a rate of 1 mg/day. A does not partition onto the sand, but B does,

with a partition coefficient of  $2E-4 \text{ m}^3/\text{kg}$ . You wish to simulate the breakthrough of the two species out the end of the column.

To simulate this system in GoldSim, you would do the following:

1. Define two species (A and B);
2. Define two media (Water and Sand) and specify their properties;
3. Define a single Pipe to represent the column;
4. Specify the properties of the Pipe;
5. Define a sink Cell and create an advective mass flux link from the Pipe to the Cell.
6. Specify the boundary condition for the Pipe; and
7. Specify the simulation settings (i.e., duration and timestep) and run the model.

The output of this simulation, in the form of time histories of the mass rate of species A and B exiting the column, is shown below:



The mean unretarded travel time,  $t$ , through a Pipe can be computed as follows:

$$t = n A L / Q S$$

where  $n$  is the porosity of the infill,  $A$  is the cross-sectional area of the Pipe,  $L$  is the length of the Pipe,  $Q$  is the flow rate and  $S$  is the fluid saturation.

In this example,

$$t = (0.3)(0.05 \text{ m}^2)(2 \text{ m}) / 1E-3 \text{ m}^3/\text{day} = 30 \text{ days}$$

As can be seen from the figure, the unretarded species (A) reaches 50% of its steady state flux rate just before 30 days (due to the impact of boundary conditions, the solution to the equation is asymmetric and the 50% breakthrough value is expected to occur slightly before the calculated mean travel time). The spread around this point is due to dispersion in the pathway. Species B reaches

50% of its steady state flux at about 60 days. This is because the effective retardation factor,  $R$ , in this particular case can be computed as:

$$R = 1 + \frac{(\rho_b)(K_d)}{n} = 1 + \frac{(1600 \text{ kg/m}^3)(2E - 4 \text{ m}^3/\text{kg})}{0.3} = 2.1$$

where  $\rho_b$ ,  $K_d$  and  $n$  are the bulk density, partition coefficient and porosity, respectively, for the Solid infill through which the fluid is flowing.

Hence, in this example, the breakthrough curve was retarded by about a factor of two.

## Defining Basic Pipe Properties

The dialog for a Pipe pathway is shown below:

The basic Pipe properties are listed on the main Pipe dialog, and are described below.

## Pipe Geometry

The first three input fields in the Pipe pathway dialog describe the overall geometry of the Pipe.

**Length:** This is the length of the pathway.

**Area:** This is the cross-sectional area of the pipe. This area includes the mobile (flowing) zone and the stagnant zone (if one is defined). It does not, however, include any areas associated with any matrix diffusion zones or coating that may be defined. If an infill medium is specified, it fills the area.

**Perimeter:** This is the wetted perimeter of the pathway. For example, if your Pipe was being used to represent a saturated fracture defined by two parallel plates 0.2 m wide and 0.001 m apart, the perimeter would be defined as 0.402 m. It is only used if you specify that the Pipe has a coating

or one or more matrix diffusion zones. If neither of these two situations apply, the input is ignored. The perimeter has dimensions of length.



**Note:** If the perimeter is specified as 0, any specified coatings and matrix diffusion zones will have no impact on the behavior of the Pipe.

## Other Basic Pipe Properties

In addition to the inputs describing Pipe geometry, Pipes require three additional inputs that control the basic behavior of the Pipe:

**Dispersivity:** This is the longitudinal dispersivity of the pathway. It has dimensions of length. The longitudinal dispersivity acts to spread or disperse species around the mean travel time as they are transported through the Pipe. Different systems disperse solutes to different degrees. A good first approximation for one-dimensional transport through a relatively homogeneous aquifer might be that the dispersivity is 10% of the total length of the pathway. You must specify a dispersivity which is greater than or equal to zero.

Note that for computational reasons, a minimum dispersivity is applied by GoldSim. The minimum value is a function of the Solution precision (specified in the Contaminant Transport tab of the Options dialog). If the precision is low, the minimum dispersivity is 2.5% of the pathway length; if the precision is medium, the minimum dispersivity is 0.5% of the pathway length; and if the precision is high, the minimum dispersivity is 0.1% of the pathway length.

Hence, if you enter a pathway length of 2000 m, and a dispersivity of 0, and the Solution precision is set to high, GoldSim will actually assume a dispersivity of 20 m (and will write a warning to the Run Log). *Because practically no real system would have a dispersivity of less than 0.1% of the pathway length, this should not pose any problems.*



**Warning:** For pathways with very low dispersivities, it will likely be necessary to adjust the solution algorithm (i.e., solution precision) in order to obtain accurate results. If the dispersivity is too low (e.g., significantly less than 1% of the pathway length), it may not be possible to obtain accurate results.

**Read more:** [Controlling the Pipe Solution Algorithm](#) (page 216).

**Infill Medium:** This is the porous medium which fills the mobile zone of the pathway. It must be an existing Solid medium in the model. You can, however, specify that there is no porous medium filling the pathway (e.g., if you were simulating a channel or river) by leaving this field blank.

The porous medium affects the behavior of the Pipe in two ways: 1) it increases the flow velocity (by reducing the effective flow area); and 2) it can act to retard any species which partition onto it.

**Fluid Saturation:** This is the degree of saturation of the Pipe. It is dimensionless, and must be greater than 0 and less than or equal to 1. If you were simulating a saturated aquifer or a river, you would specify the fluid saturation as 1 (the default). If, however, you were simulating flow through an unsaturated porous medium (e.g., surface soils or a vadose zone), this would be specified as less than 1.

Decreasing the fluid saturation has the same effect as decreasing the porosity of the porous infill medium: 1) it increases the flow velocity (by reducing the effective flow area); and 2) it increases the degree of retardation due to partitioning onto the porous infill and coating media (by reducing the effective volume of fluid present in the pathway relative to these solids).

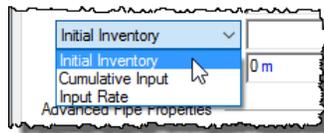
### Defining Initial/Boundary Conditions for a Pipe

There are two ways by which species mass can enter a Pipe:

- Through a mass flux link from another pathway to the Pipe; and/or
- By defining an initial condition and/or a boundary for the Pipe.

In this section, we discuss defining an initial and/or boundary condition for a Pipe.

An initial condition/boundary condition for a Pipe is specified using the drop-list directly below the Discrete Changes field within the Pipe dialog. This drop-list provides three options:



- **Initial Inventory.** This is the default, and represents the initial inventory of each species (at the beginning of the Pipe). This field only accepts vectors by species with dimensions of mass. Moreover, this input cannot be specified as a function of time (if it is, GoldSim will display a fatal error when you try to run the model).
- **Cumulative Input.** This option provides a mechanism for simultaneously specifying an initial condition and a rate of mass addition (that may change with time). This field only accepts vectors by species with dimensions of mass. It represents the *cumulative* amount of mass of each species added to the Pipe at a given time. Hence, if it is constant, it represents an initial condition. If it increases with time, its rate of change represents a specified rate of addition. Correct use of the "Cumulative Input" is summarized in the table below:

To specify this:	Enter the following into the "Cumulative Input" field:
An initial condition (at the beginning of the Pipe)	A constant vector with dimensions of mass (in this case, however, it would be more transparent to use the "Initial Inventory" option).
An initial condition and a <i>constant</i> rate of addition	An expression such as: $Initial + Rate * Etime$ , where Initial is a constant vector (with dimensions of mass) and Rate is a constant vector (with dimensions of mass/time).
An initial condition and a <i>time-variable</i> rate of addition	The output of a Pool, Reservoir or Integrator element (with output dimensions of mass) with a specified Initial Value and (time-variable) Rate of Change.



**Warning:** The Cumulative Input must stay constant or increase with elapsed time. That is, you cannot remove mass from a Pipe using the Cumulative Input field. If the value ever begins to decrease with time, a fatal error occurs.

- **Input Rate.** The third option is used to specify a rate of mass addition (that may change with time). This field only accepts vectors by species with dimensions of mass/time. It represents the rate at which mass of each species is added to the Pipe over the next timestep.



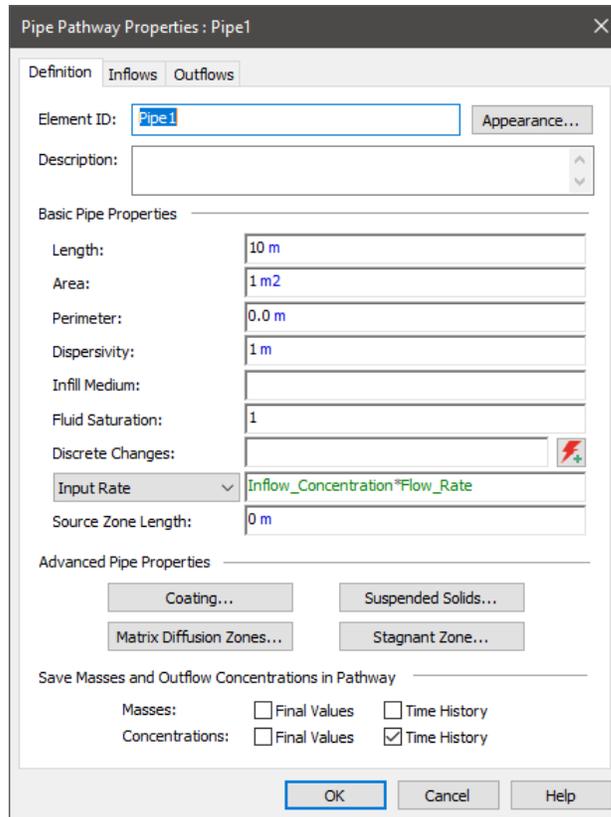
**Note:** One way to easily enter a vector of data into an input field without having to create a separate element is to use GoldSim's vector constructor function. For example, entering "vector(1g)" into the Cumulative Input field results in an initial condition of 1 g of each species being present in the Pipe.

Although the **Input Rate** and **Cumulative Input** options provide a quick and convenient way to enter mass input rates, if mass input rates into a Pipe are changing with time (e.g., because the inflow concentration is changing), a slightly more accurate way (both numerically and conceptually) to specify such a boundary condition is to create a "Source Cell" that is defined using a **Defined Concentration**.

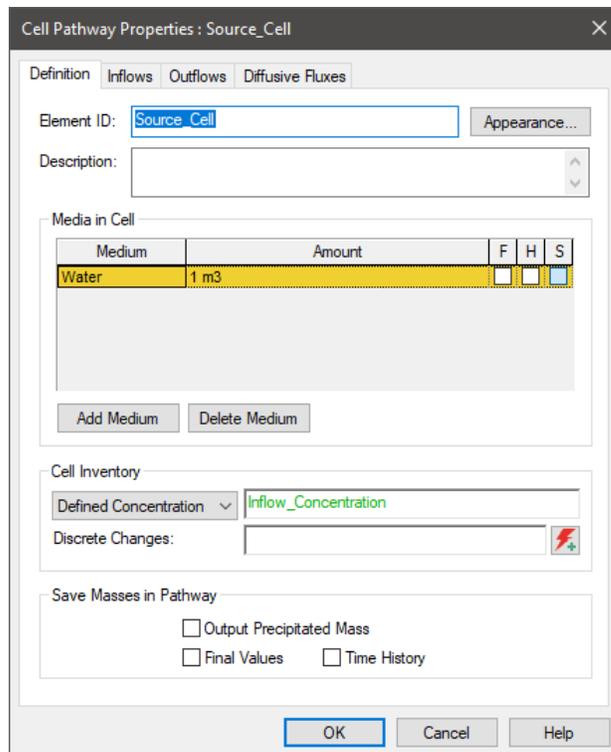
**Read more:** [Defining Initial and/or Boundary Conditions for a Cell](#) (page 126).

As an example, consider a case in which you have a boundary condition with a constant inflow rate (Flow\_Rate) and a time-varying Inflow\_Concentration. The Pipe has a constant outflow rate (equal to the inflow rate). You could model this in two ways:

- In the first approach, you simply provide an **Input Rate** to the Pipe:

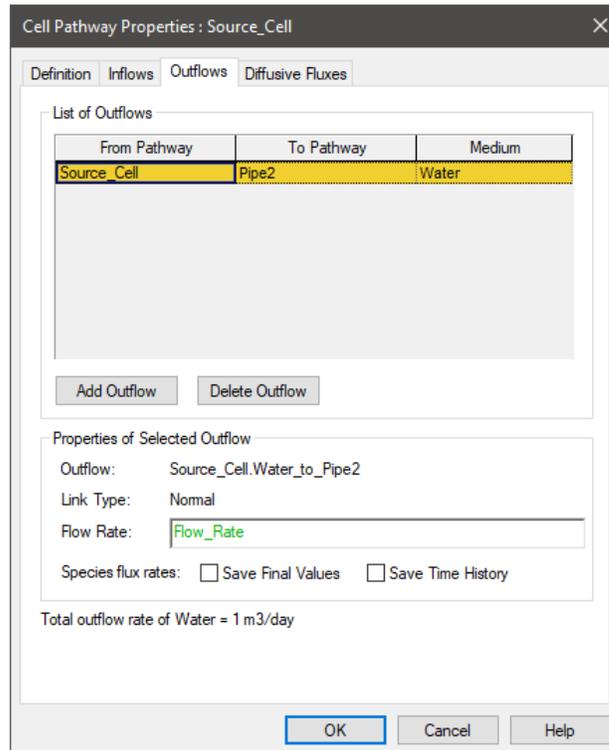


- In the second approach, you define a “Source\_Cell” that looks like this:



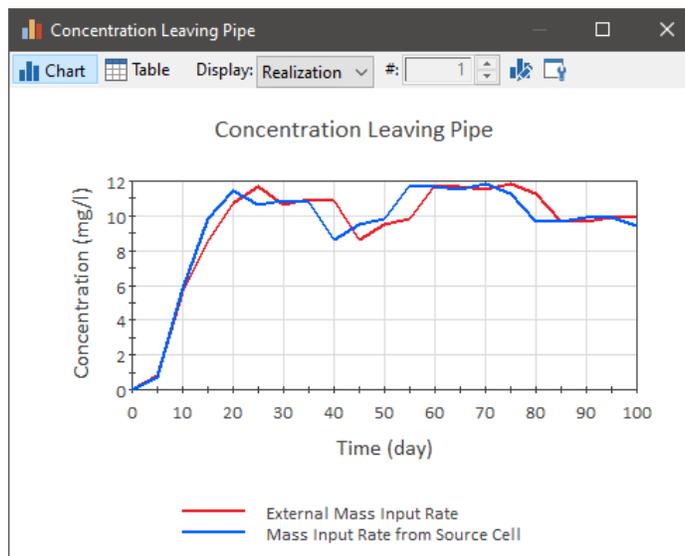
The volume is set to an arbitrarily small number (it is not used to compute concentrations since the concentration is fixed). A **Defined**

**Concentration** is specified for this Source\_Cell that will flow into Pipe. That is, the Source\_Cell has an outflow to the Pipe:



The Pipe itself has no **Input Rate** specified.

If we run this model (for 100 days with a 5 day timestep) and compare the results for these two different approaches to representing the boundary condition (in terms of the concentration leaving the Pipe), they look like this:



What we see is that the mass that is input “externally” (using the **Input Rate**) lags by one timestep. This is because in this, due to the way the external boundary condition must be applied when solving the pathway equations, a one timestep lag is introduced. Hence, the second approach is a more accurate representation (although for a small timestep, the differences would likely be

### Simulating Discrete Changes to the Mass Inventory in a Pipe

insignificant). Conceptually, however, this is a bit more accurate way to represent the boundary condition (since the boundary condition is actually treated as part of the pathway network).

In addition to adding mass to a Pipe via an initial/boundary condition, and adding/removing mass via mass flux links, GoldSim allows you to instantaneously add species mass to a Pipe.

This is done using the Discrete Changes field in the Pipe dialog, which is located toward the bottom of the “Basic Pipe Properties” section:



This field only accepts discrete change signals. (Discrete change signals are discussed in detail in "Simulating Discrete Events" in the **GoldSim User's Guide**.) The discrete change signal must be a vector by species and have dimensions of mass. Typically, such a discrete change signal will be the output of a Discrete Change element that has been triggered by an event.

Discrete change signals have an *instruction* associated with them. Two types of instructions are possible: Add and Replace. The Discrete Changes field for a Pipe only accepts Add signals.

When an Add signal is sent to a Pipe during a simulation, the specified amount of mass of each species in the discrete change vector is added to the current mass in the pathway.



**Note:** The discrete change vector cannot contain negative numbers (i.e., you can NOT discretely remove mass from a Pipe; you can only add mass).

Like most input fields that accept discrete change signals, you can specify multiple discrete changes. You can do this in two ways:

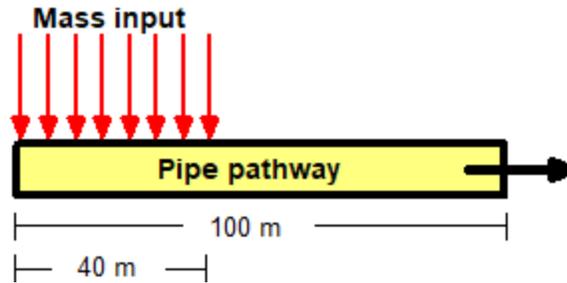
1. You can enter multiple discrete changes into the input field by separating the entries using a semi-colon; and
2. You can use the Multiple Discrete Changes button to the right of the input field (i.e., the small button with two exclamation marks) to access a table listing the Discrete Changes (to which you can add or delete entries).

In the latter case, any Discrete Changes which are added to the list are also automatically added to the input field, separated by semi-colons.

The Discrete Changes field can be very useful for instantaneously modifying your system in response to discrete events. Note, however, that this feature should be used with care, since when it is applied, conservation of mass in the system is the responsibility of the user.

### Controlling How Mass Enters a Pipe

GoldSim allows you to control the manner in which mass enters a Pipe. In particular, you can specify the **Source Zone Length** parallel to the flow direction in the pathway. Hence, if your pathway had a length of 100m, and you specified a **Source Zone Length** of 40m, mass would enter the pathway uniformly over the first 40m (rather than at the beginning of the pathway):



This is useful, for example, if your Pipe represents an aquifer which is being loaded from above with mass from source which is of such an areal extent (e.g., a landfill) that it extends over a significant portion of the pathway and therefore cannot be treated as a point source.

By default, the **Source Zone Length** for a Pipe is zero. In this case, any mass entering the Pipe is treated as a point source which is applied at the beginning of the Pipe. If the **Source Zone Length** for a Pipe is greater than zero, the mass is distributed uniformly over the specified length.

Two points regarding the use of the **Source Zone Length** are worth noting:

- The **Source Zone Length** is applied to all forms of mass that enter the Pipe: mass that enters as an initial or boundary condition, mass that enters the Pipe from other pathways via a mass flux link, and mass that enters the Pipe as a specified discrete change via the **Discrete Changes** field.
- If the **Source Zone Length** is larger than the Pipe **Length**, the **Source Zone Length** is assumed to be equal to the Pipe **Length** (and a warning message is written to the Run Log).



**Warning:** The Source Zone Length should only be used if the total flow in the Pipe is substantially larger than the flow associated with the incoming mass. This is because that the Source Zone Length does not change the flow rate along the Pipe; it only impacts where the mass is input. Hence, it is equivalent to assuming that the amount of flow associated with the mass entering the pathway is negligible relative to the total flow in the pathway (e.g., associated with “clean” upgradient water).

## Defining a Sorptive Coating Material for a Pipe

You can define a coating medium for a Pipe which can act to retard transport through the pathway. This might be appropriate, for example, if you were simulating flow through a fracture which had a coating around the perimeter. The mobile fluid in the pore volume of the pathway, the immobile fluid within the coating material, the infill material and the coating material are all assumed to be at equilibrium at all times with respect to the partitioning of species.

You define a coating material via the **Coating...** button on the Pipe dialog. When you press this button, the following dialog is displayed:

The **Coating Medium**, if specified, must be an existing Solid medium in the model. If there is no coating medium in the pathway, you should leave this field blank (the default). The **Coating Thickness** specifies the thickness of the coating material along the perimeter, and has dimensions of a length.

The mass of Coating Medium per unit length of pathway (which impacts the degree to which the coating retards species) is simply the product of the Coating Thickness, the pathway Perimeter and the density of the Coating Medium.



**Note:** If the perimeter or the coating thickness is specified as 0, the coating material will have no impact on the behavior of the Pipe.

## Simulating Storage Zones in a Pipe

In addition to the linear retardation mechanisms associated with infill and coating materials, Pipes can also represent interchanges with *immobile storage zones* along the length of the pathway. These exchange processes act orthogonal to the flow direction. The approach of representing such storage zones was originally developed for modeling fracture flow with matrix diffusion, but has also been used to model flow through porous media.

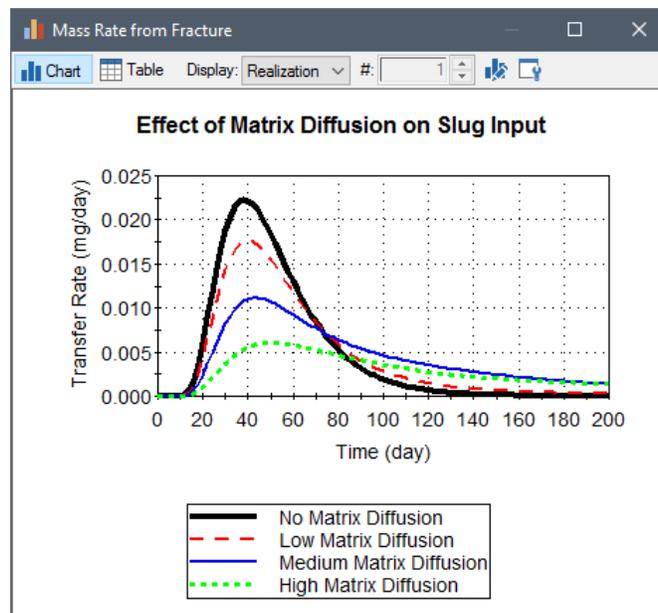
Pipes can represent two types of storage zones:

- matrix diffusion zones; and
- a “stagnant” dispersive zone.

## Understanding Matrix Diffusion Zones

Matrix diffusion is the process by which solutes diffuse from a mobile zone (e.g., a fracture) into surrounding porous matrix material. In GoldSim, it is assumed that this diffusive process is one-dimensional and orthogonal to the flow direction.

The figure below illustrates the effect of matrix diffusion on the breakthrough of a slug input. Note that as the degree of matrix diffusion increases (implemented in this case by increasing the perimeter, and hence the diffusive area), the breakthrough is retarded and the tail is extended far to the right.



GoldSim allows up to three separate matrix diffusion zones to be specified for each Pipe. The fraction of the pathway’s perimeter associated with each zone is

specified by the user. Each matrix diffusion zone is also assigned a thickness (which can be defined to vary over the pathway perimeter). For each zone, one of three possible one-dimensional diffusive geometries can be assumed:

- *slab* (in which the diffusive area remains constant with distance into the matrix). Such a model could be appropriate, for example, for representing uniform, parallel fracture sets, in which the thickness of the zone was defined as half the thickness of the rock block (assuming that a similar fracture exists on the other side of the rock block).
- *sphere* (in which the diffusive area decreases with distance into the matrix according to a spherical geometry). Such a model could be appropriate, for example, to represent intact blocks in highly fractured zones.
- *slot* (in which the diffusive area increases exponentially with distance into the matrix). Such a model could be appropriate, for example, to represent a long, “thin” (width  $\ll$  length) pathway.

Each matrix diffusion zone is assigned a porous material type (a Solid), and the properties of this medium impact the transport properties (diffusivity, partitioning) within the zone.

A **skin zone** can also be defined for the Pipe. The skin zone is defined in a similar manner to that of the matrix diffusion zones (although its geometry is always assumed to be slab). While the three matrix diffusion zones exist in parallel, the skin zone, if present, is assumed to exist *in front* of all matrix diffusion zones (i.e., between the matrix diffusion zones and the mobile zone). Hence, if a skin zone is present, species must first diffuse through the skin before reaching the underlying diffusive zones (forming a two-layer diffusive system).

### **Pipe Pathway Example #2: Matrix Diffusion Zones**

To illustrate the use of matrix diffusion zones, let's consider a simple example. This particular example file, Pipe2\_MatrixDiffusion.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

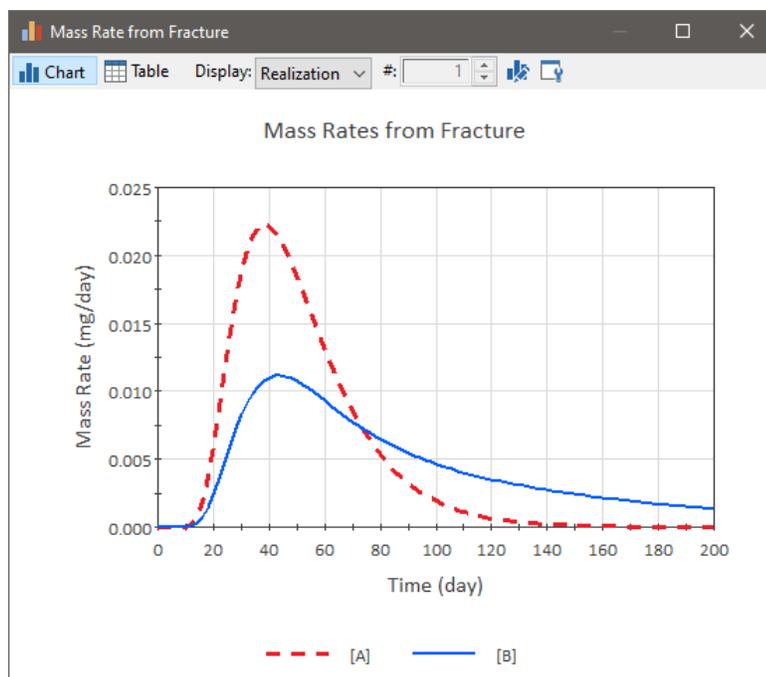
In this example, we wish to simulate a tracer test in which we inject two tracers into a single fracture in a rock block. The fracture is 2 m long, 0.5 m wide and has an aperture of 1 mm. Water flows through the fracture (which is saturated) at a rate of  $2E-5$  m<sup>3</sup>/day. The dispersivity (in the absence of matrix diffusion) for the fracture is assumed to be 0.2 m. 1 mg of species A and B are injected into the fracture. A 10 cm thick matrix diffusion zone (with a porosity of 0.01) exists in the rock matrix on either side of the fracture. Species A, however, can not diffuse into the rock (it is too large).

To simulate this system in GoldSim, you would do the following:

1. Define the two species and define their properties (particularly the relative diffusivities);
2. Define two media (Water and Rock) and specify their properties;
3. Define a single Pipe to represent the fracture;
4. Specify the properties of the Pipe;
5. Define a sink Cell and create an advective mass flux link from the Pipe to the Cell.
6. Specify the initial condition for the Pipe; and

- Specify the simulation settings (i.e., duration and timestep) and run the model.

The output of this simulation, in the form of time histories of the mass rate of species A and B exiting the fracture, is shown below:



Note that species B, which can diffuse into the rock matrix, has a long "tail" indicative of the matrix diffusion process. Species A, which was not allowed to diffuse into the matrix, is unaffected (and controlled only by the advective-dispersive process).

### Defining Matrix Diffusion Zones

Matrix diffusion zones are defined via the **Matrix Diffusion Zones...** button on the Pipe dialog. When you press this button, the following dialog is displayed:

Used	Medium	Geometry	Minimum Thickness	Maximum Thickness	Fraction of Perimeter	Effective Area (m2)
<input checked="" type="checkbox"/>	Rock	Slab	0.1 m	0.1 m	1.0	0.05 m2
<input type="checkbox"/>		Slab	0.0 m	0.0 m	1.0	
<input type="checkbox"/>		Slab	0.0 m	0.0 m	1.0	

You can specify up to three matrix diffusion zones having different properties. The zones are activated by the check boxes. Inactive zones are grayed out.

The user can define up to three matrix diffusion zones. Clicking the **Used** checkbox to the left of each zone activates ("turns on") the zone. A lower zone can only be activated if the zone above it is active. Inactive (unused) zones are grayed out (and are not represented in the model).

For each zone, it is necessary to define a **Medium**, a **Geometry**, a **Minimum Thickness**, a **Maximum Thickness**, and a **Fraction of Perimeter**:

**Medium:** This is the porous medium for the matrix diffusion zone. It must be a previously defined Solid medium.

**Geometry:** This is the assumed diffusive geometry for the matrix zone. There are three options: Slab, Sphere, and Slot.

**Read more:** [Understanding Matrix Diffusion Zones](#) (page 206).

**Minimum Thickness and Maximum Thickness:** These two inputs define the thickness of the matrix diffusion zone. They have dimensions of length. The Maximum Thickness must be greater than or equal to the Minimum Thickness (otherwise it is ignored and only the Minimum Thickness is used). GoldSim assumes that the thickness of the zone varies uniformly over the pathway perimeter between the specified minimum and maximum values, such that every part of the pathway perimeter “sees” the full range of matrix thicknesses. Mathematically, this is represented in GoldSim by integrating the mobile to immobile zone flux for each of the matrix diffusion zones over the specified range of thickness (for more details, see Appendix B).

**Fraction of Perimeter:** This is the fraction of the pathway's perimeter which is connected to this particular matrix diffusion zone. It is dimensionless, and must be greater than or equal to 0. It can, however, be greater than 1 (implying the perimeter with respect to matrix diffusion is larger than specified in the Pipe's main dialog).

For each zone, GoldSim internally computes the **Effective Area** and displays it to the right of each matrix diffusion zone. This represents the area in a cross-section perpendicular to the flow direction. By comparing this area to the specified pathway area, the user can better determine whether the diffusive geometry and thickness for the zone have been defined reasonably.

You can also define a diffusive skin for the pathway:

**Skin medium:** This specifies the Solid medium which is the "skin" material for the pathway, and is optional (i.e., the field can remain empty), . The skin medium must be a previously defined Solid medium. The skin is a diffusive layer in contact with the mobile zone. If a skin is specified, species must diffuse through the skin before entering any of the matrix diffusion zones (i.e., the skin, if defined, is between the matrix diffusion zones and the mobile zone).

**Skin Thickness:** This defines the thickness of the skin for the pathway, and has dimensions of length. If no Skin Medium is specified, this field is ignored. The Skin Thickness must be greater than or equal to zero.

### ***Understanding the Stagnant Dispersive Zone***

A stagnant dispersive zone represents another type of immobile storage zone (in addition to a matrix diffusion zone) that can act to disperse solute transport in a Pipe.

The stagnant dispersive zone was designed to be used to represent the low-velocity or “stagnant” pores or regions within the plane of a fracture, or within a porous medium. Such zones are likely to exist in many types of subsurface systems. For example, for an aquifer under a uniform head gradient, the seepage velocity varies with the square of pore aperture, so in a medium with variable pore sizes it is possible for smaller pores to have a very low velocity, and hence act as a sort of storage zone.

For this kind of storage zone, interchange between the mobile zone and the storage zone may actually occur by both advective and diffusive processes. For relatively high gradient, short-term systems (such as those associated with tracer

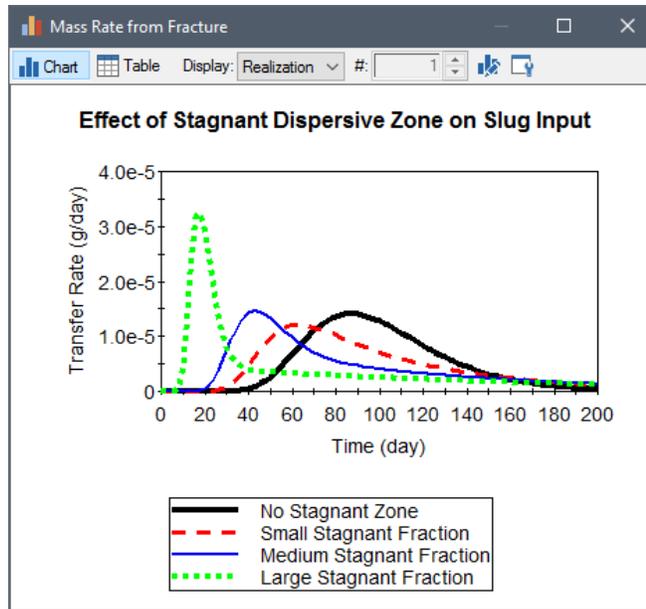
tests), the advective interchange will typically dominate the system, whereas for longer time periods under lower gradients the diffusive exchange process may dominate. (As represented in GoldSim, however, only advective exchange between the stagnant and the mobile zone is simulated.)

Note that it is actually this type of physical model that is represented when a classic “dispersivity” factor is used to describe solute dispersion. In reality, there is a continuum of velocities within a pathway (i.e., a continuum of “dispersive storage zones”). The classic dispersivity parameter is simply a factor that corrects for the fact that we typically model flow at a macro-scale, rather than a micro-scale (in which all of the dispersive zones are explicitly represented).

GoldSim allows the user to explicitly represent a single stagnant dispersive zone in a one-dimensional pathway. The user must specify the fraction of the pathway which is assumed to be “stagnant”. As noted by its name, this portion of the pathway is assumed to have negligible advective velocity. It can be filled with a porous medium (to which species can sorb), which may be different from that in the mobile zone of the pathway (i.e., the infill medium). Transfer between the stagnant zone and the mobile zone is advective, and thus varies proportionately to the quantity of fluid flowing through the pathway. The constant of proportionality (referred to herein as the *transfer rate*), has dimensions of inverse length, and is defined as the probability of an individual solute molecule moving from the mobile zone to the stagnant zone, per length of distance traveled in the mobile zone.

Because the transfer rate is proportional to the flow rate in the pathway, this type of mobile-storage zone transfer is qualitatively different from transfer between the mobile zone and matrix diffusion zones. A stagnant dispersive zone acts to disperse solute flowing in the pathway in a unique manner. In the limit where the product of the transfer rate and the pathway length is much greater than one, a stagnant dispersive zone produces a dispersion profile identical to that associated with the conventional advection-dispersion equation. However, if this product is not significantly greater than one, it produces a highly asymmetric dispersion profile, characterized by a sharp leading edge and an elongated tail in the breakthrough curve (similar to that resulting from the presence of matrix diffusion zones).

The figure below illustrates the effect of a stagnant dispersive zone on the breakthrough of a slug input (in this case, the product of the transfer rate and pathway length is less than 1).



Note that if the total area and the flow rate of the pathway is held constant while the fraction of the pathway which is stagnant is increased (as in the figure shown above), the mean breakthrough curve is actually shifted to the left (shorter times), since the effective area of the mobile zone is decreased, and hence the velocity in the path is increased.

### Defining a Stagnant Dispersive Zone

The stagnant dispersive zone is defined via the **Stagnant Zone...** button on the Pipe dialog. When you press this button, the following dialog is displayed:

Clicking the **Use Stagnant Zone** checkbox activates ("turns on") the zone. If this checkbox is cleared, the Stagnant Zone inputs are grayed out (and are not represented in the model).

The Stagnant Zone requires three inputs: the **Stagnant zone infill medium**, the **Fraction of area which is stagnant**, and the **Transfer Rate into stagnant zone**:

**Stagnant zone infill medium:** This is the porous medium in the stagnant zone. If defined, it must be a previously defined Solid medium (the stagnant zone need not contain an infill medium).

**Fraction of area which is stagnant:** This is the fraction of the pathway cross-sectional area occupied by the stagnant medium. It is dimensionless and must be greater than or equal to 0 and less than 1.

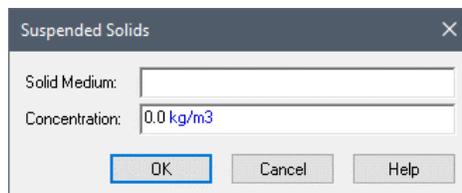
**Transfer rate into the stagnant zone:** This is the equilibrium exchange rate from the mobile zone to the stagnant zone, and has dimensions of inverse length. It is defined as the probability of a dissolved molecule in the

## Simulating Suspended Solids in a Pipe

mobile zone entering the stagnant zone, per unit length traveled in the mobile zone. It cannot be negative.

GoldSim allows you to specify that suspended Solids are present in the Pipe. These Solids are assumed to be advected and dispersed along the Pipe, but are not subject to retardation processes or interactions with storage zones. Species which partition onto the suspended Solids are transported with them as they move through the Pipe.

Suspended solids are specified to be present in the Pipe via the **Suspended Solids...** button on the Pipe dialog. When you press this button, the following dialog is displayed:



A Pipe can have a single suspended Solid for which you must define the **Solid Medium** and the **Concentration**:

**Solid Medium:** This is the solid suspended in the Pipe. It must be a previously defined Solid medium.

**Concentration:** This is the concentration of the suspended solid in the Pipe fluid. It has dimensions of mass per volume.

Suspended solids in a Pipe can increase the "carrying capacity" of the water in the mobile zone, by allowing solute species to sorb onto and be transported by particulates. This has the effect of reducing retardation due to sorption onto infill material and coating, as well as the effects of any matrix diffusion or stagnant zones which have been defined. Mathematically, suspended solids in a Pipe can be thought of as increasing the effective concentration in the pathway fluid, thereby increasing the mass flux of species out of the Pipe. In particular, assuming no dispersion, the advective mass flux of species  $i$  leaving the Pipe,  $\text{Flux}_i$ , becomes:

$$\text{Flux}_i = Q \text{cd}_i (1 + K_i V_{\text{susp}} c_{\text{susp}})$$

where  $Q$  is the flow rate in the Pipe (volume/time),  $\text{cd}_i$  is the dissolved concentration of species  $i$  (mass/volume),  $K_i$  is the partition coefficient for species  $i$  for the suspended solid medium (volume/mass),  $c_{\text{susp}}$  is the suspended solid concentration (mass/volume), and  $V_{\text{susp}}$  is the dimensionless Advective Velocity Multiplier for the suspended Solid (a property of the Solid).

**Read more:** [Advanced Solid Properties](#) (page 77).



**Note:** The suspended solid concentration only impacts advective mass flux links leaving the Pipe and does not have any impact on the diffusion of particulates into the Pipe. That is, if a diffusive mass flux link is created between a Cell containing a suspended solid and a Pipe containing the same suspended solid, for the purpose of simulating the diffusive flux of particulates, the concentration of particulates on the Pipe side of the link is assumed to be zero.

**Read more:** [Flux Links to/from Pipes](#) (page 214).

## Pipe Pathway Outputs

Pipe pathways have at least two outputs:

- **Mass\_in\_Pathway.** This is a vector by species with dimensions of mass. It represents the total mass of each species in the Pipe.



**Note:** The Laplace transform algorithm for Pipes directly computes the flux rate leaving the Pipe. In order to track the amount of mass in the Pipe, we assume that the mass enters or exits the Pipe at a uniform rate over the timestep. If you use a large timestep and/or there is low dispersivity, this assumption may not be appropriate, and this can result in small errors in the amount of mass reported in the Pipe. This assumption does not affect the accuracy of the Pipe discharges, just the value of the reported amount of mass in the Pipe.

---

- **Concentration.** This is a vector by species with dimensions of mass per volume. It represents the concentration of each species in the Reference Fluid at the point where it exits the Pipe. This is a “total concentration”, and includes species sorbed onto suspended solids.



**Note:** The computed concentration is an approximation, equal to the mass outflux divided by the flow rate. Because the mass flux includes a dispersive component, the concentration will be slightly overestimated during periods of increasing concentrations, and slightly underestimated during periods of decreasing concentrations.

---

In addition, for every advective mass flux link in which the Pipe is the Outflow (upstream) pathway, an output is created on the Pipe:

- **Medium\_to\_Path2**, where *Medium* is the name of the flowing medium, and *Path2* is the name of the linked (Inflow) pathway. This is a vector by species, and has dimensions of mass/time. It represents the mass flux of each species from the Pipe to the downstream pathway.

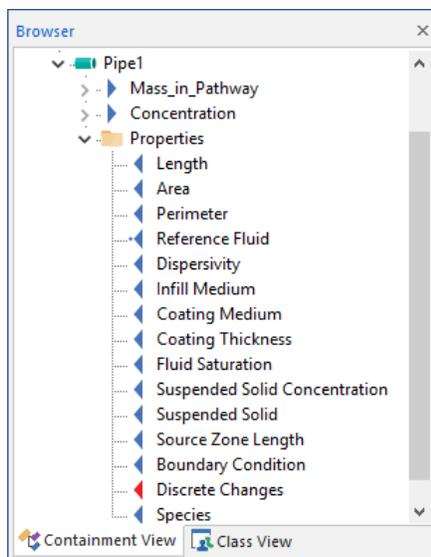
**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94).

It is important to understand that the mass flux outputs from a Pipe represent the mass rate over the *previous* timestep. This can have implications if you choose to integrate one of these outputs (using an Integrator).

**Read more:** [Manipulating Pathway Outputs](#) (page 253)

## Viewing a Pipe in the Browser

The browser view of a Pipe pathway is shown below:



The Properties folder contains all the inputs for the Pipe. If Matrix Diffusion or Stagnant Zones exist, subfolders are added for these. The Inflows and Outflows folders contain all of the mass flux links for the Pipe.



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

The pathway's mass and concentration outputs are listed first. Note that for a Pipe, the concentration always refers to that in the Reference Fluid.

The Properties folder contains the basic inputs for the Pipe, including the two subfolders containing the matrix diffusion zone and stagnant zone properties. (Note that these subfolders are not shown if these zones are not being simulated.) With two exceptions (listed below), you can create a link to any of these property inputs using the Link Cursor.

Note that the Species input and the Reference Fluid input also appear in the Properties folder. The Species input is automatically linked to the nearest Species element when the Pipe is created. Similarly, the Reference Fluid input is automatically linked to the nearest Reference Fluid element when the Pipe is created. *These links cannot be changed using the Link Cursor, and are displayed for information purposes only.*

If the Pipe has any mass flux links associated with it, the corresponding inputs and outputs for these links are organized into the Inflows, Outflows, and Diffusive Influxes folders. These folders are not shown if they are empty.

**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94); [Inputs and Outputs Associated with Diffusive Mass Flux Links](#) (page 101); [Inputs and Outputs Associated with Direct Transfer Mass Flux Links](#) (page 105); [Inputs and Outputs Associated with Precipitate Removal Mass Flux Links](#) (page 110); [Inputs and Outputs Associated with Treatment Mass Flux Links](#) (page 116).

## Flux Links to/from Pipes

The only way to transport mass *out* of a Pipe is by specifying an advective mass flux link to another pathway. Diffusive mass flux links (diffusive outfluxes),

and special purpose mass flux links (direct transfer, precipitate removal and treatment) *from* Pipes cannot be created.

**Read more:** [Understanding Advective Mass Flux Links](#) (page 90).

Advective mass flux links are used to transport mass via a flowing medium. Mass which is dissolved, suspended or otherwise associated with the flowing medium is transported with the medium as it moves. For Pipe pathways, the flowing medium is always the Reference Fluid.

You can transport mass *into* a Pipe via an advective mass flux link from any other type of pathway and/or via a diffusive mass flux link from a Cell pathway. Within GoldSim, the concentration and diffusive length on the Pipe side of a diffusive mass flux link are assumed to be zero. Hence, like advective mass flux links, diffusive mass flux links involving Pipes are uni-directional.



**Warning:** GoldSim does not enforce a balance for the flow of the Reference Fluid in a Pipe. That is, the Inflows into a Pipe do not need to be equal to the Outflows from the Pipe. If the specified Outflows are greater than the specified Inflows, conceptually the effect on the species concentrations leaving the Pipe is one of dilution, since "clean" fluid is assumed to be flowing into the Pipe. If, however, the specified Outflows are less than the specified Inflows, in the absence of decay and dispersion, the species concentrations leaving the Pipe would be greater than those entering the Pipe. Conceptually, GoldSim would assume that a quantity of "clean" fluid (carrying no species mass) flowed out of the Pipe in order to conserve the flow rate and volume in the Pipe. Although there are some physical situations in which you may actually want to do this (e.g., in order to simulate the evaporation of Water from a Pipe), typically such behavior would not be intended. As a result, whenever the Inflows to a Pipe exceed the Outflows, GoldSim provides a (non-fatal) warning message to the Run Log.

**Read more:** [Mass Balance of Transport Media in Pathway Networks](#) (page 253).

### ***Advection and Diffusion of Particulates to/from Pipes***

Suspended solids can advect and diffuse into Pipes, and can advect out of Pipes (mass cannot diffuse out of Pipes).

Suspended solids can advect into a Pipe from another pathway containing suspended solids. Suspended solids can also diffuse into a Pipe from a Cell or Aquifer containing suspended solids. The species mass associated with the suspended solids in the upstream (Outflow or Outflux) pathway enter the Pipe regardless of whether suspended solids are specified as being present in the Pipe. When suspended solids (carrying species mass) enter a Pipe from another pathway, conceptually, the particulates are assumed to immediately disintegrate upon entering the Pipe (releasing their species mass to the fluid in the Pipe). If suspended solids are present in the Pipe, the species mass will then partition onto these solids.

**Read more:** [Advection of Particulates to/from Cells](#) (page 138); [Diffusion of Particulates to/from Cells](#) (page 141).

### ***Simulating Time-Variable Pipe Properties***

The central concept of the Laplace transform solution technique used by GoldSim to simulate transport through Pipes is that the discharge history is a linear (and time invariant) function of the input history (for details on the Laplace transform solution, see Appendix B, "Details of Pathway Computations").

Because the Laplace transform approach requires that the transport equations be linear and unchanging in time, if any of the properties of a Pipe (e.g., partition coefficients for solid media, area, perimeter, storage zone properties) change during a realization, GoldSim must use an approximation to represent this change.

In particular, when a change in the properties of a Pipe occurs, *the change has no effect on mass that was already in the pathway* prior to the change. Mass which is already in the pathway continues to be transported based on the properties at the time it entered the pathway. Only mass that enters the pathway subsequent to the change is affected and utilizes the updated properties.

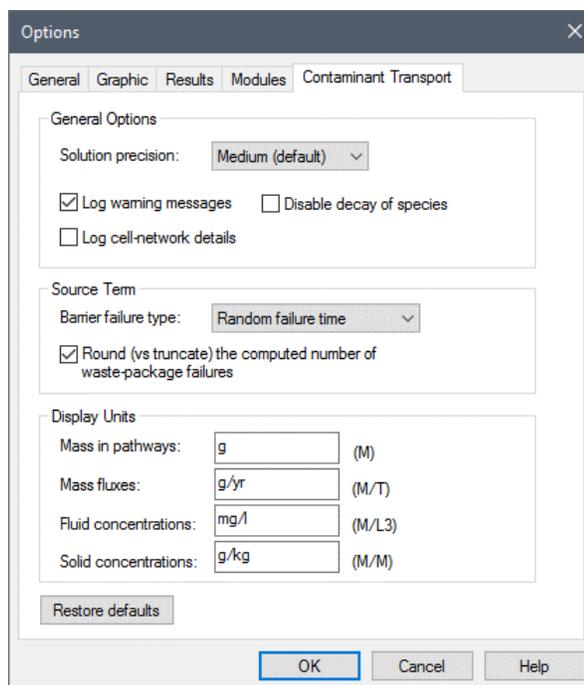
Hence, if you are simulating a Pipe which is long (i.e., has long travel times for some species) and has properties that vary significantly over time, this approximation can result in errors. In such a case, the way to minimize these errors is to discretize long pathways into a series of shorter pathways (such that travel time through each Pipe pathway is relatively rapid).



**Note:** If you do discretize a long pathway into a series of shorter Pipes, the dispersivity (which is typically defined as a fraction of the length of a pathway) should be defined in terms of the total length (not the length of each individual Pipe).

## Controlling the Pipe Solution Algorithm

There is one aspect of the solution algorithm that you may need modify in order to increase the accuracy of simulations using Pipes. This feature is accessed via the Contaminant Transport tab in the Options dialog (accessed from the main menu items **Model | Options...**):



GoldSim uses a particular algorithm (the de Hoog algorithm) to carry out the Laplace transform calculations. This algorithm includes a parameter which controls the number of terms used in an approximation within the solution. The number of terms used is determined by the **Solution precision** field in the Options dialog (note that this field also controls the precision of the Cell

pathway algorithm). There are three possible choices for the solution precision (Low, Medium, High). If Medium is selected (the default), GoldSim uses 15 terms in the Laplace transform solution. If Low is selected, it uses 5; if High is selected, it uses 25. You only need be concerned with this value if you are trying to simulate Pipes with very low dispersivity values. In such a case, you may need to select High precision (i.e., 25 terms) in order to reduce oscillations in your computed fluxes. The solution algorithm for Pipes is discussed in detail in Appendix B (in a section entitled *Solution Technique for Pipe Pathways*).

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

## Summary of Limitations on the Use of Pipe Pathways

While Pipe pathways are versatile and powerful, they do have several limitations, which are worth summarizing here:

- Unlike Cell and Aquifer pathways, GoldSim does not apply solubility limits within Pipe pathways.
- If the properties of a Pipe (e.g., partition coefficients, flow rates) change as a function of time, GoldSim has to use an approximation. The approximation is that species are discharged from a pathway based on the properties of the pathway (and the outflow rate) *at the time the species (or their parents) entered it*.
- Pipe pathways with very low dispersivities ( $\ll 1\%$  of the pathway length) can produce unstable and inaccurate results (even if using a High **Solution precision**).

Two additional limitations (that has not been discussed previously) are as follows:

- Pipe pathways with transit times which are much less than a single timestep can produce unstable and inaccurate results. In such a case, a High **Solution precision** may be necessary to keep the solution stable and accurate.

**Read more:** [Controlling the Pipe Solution Algorithm](#) (page 216).

- “Looping” reaction chains (A decays to B and B decays to A) are not permitted. Defining such reaction loops in a model that uses a Pipe will result in a fatal error message.

If any of these limitations applies, then the Aquifer pathway may be preferred over the Pipe pathway.

**Read more:** [Using Aquifer Pathways](#) (page 174).

## Saving Results for a Pipe

Pipe pathways produce the following outputs:

- the total mass of each species in the pathway;
- the concentration of each species in the Reference Fluid exiting the pathway; and
- the mass flux of each species for any specified advective Outflows.

These outputs are all vectors by species. Reference Fluid concentrations have dimensions of mass/volume. Fluxes have dimensions of mass/time.

You specify that you wish to save these results in two different places:

You specify that you wish to save these results in two different places:

1. Species masses in the pathway and concentrations in the Reference Fluid exiting the pathway are saved by clicking **Final Values** and/or **Time History** at the bottom of the Pipe editing dialog:

Save Masses and Outflow Concentrations in Pathway			
Masses:	<input checked="" type="checkbox"/> Final Values	<input checked="" type="checkbox"/> Time History	
Concentrations:	<input checked="" type="checkbox"/> Final Values	<input checked="" type="checkbox"/> Time History	

- Fluxes are saved by selecting a mass flux link in the Inflows or Outflows tab for a linked pathway and clicking **Save Final Values** and/or **Save Time History** at the bottom of the dialog:

Properties of Selected Outflow	
Outflow:	Aquifer.Water_to_Downstream_Cell
Link Type:	Normal
Flow Rate:	<input type="text" value="1 m3/day"/>
Species flux rates:	<input checked="" type="checkbox"/> Save Final Values <input checked="" type="checkbox"/> Save Time History

If you are running multiple realizations, the Time History box is ignored, and unless an output of the element is connected to a Time History Result element, no time history results will be saved at all for the element. In fact, in such a case, the Save Results section would look like this:

Final Values  Monte Carlo Histories

In this particular case, because the simulation involves multiple realizations, the “Time History” checkbox is replaced by a “Monte Carlo Histories” checkbox. This checkbox is grayed out, since it is only used for information purposes. You cannot edit it directly, and its appearance is completely determined by whether or not the output is connected to a Time History Result element. That is, in order to save time history results for a Pipe output when running multiple realizations, you must connect it to a Time History Result element.

The display units for masses, concentrations and fluxes for all pathways are specified in the **Contaminant Transport** tab of the Options dialog (accessed via **Model | Options...** from the main menu):

Options	
General   Graphic   Results   Modules   <b>Contaminant Transport</b>	
General Options	
Solution precision:	Medium (default) v
<input checked="" type="checkbox"/> Log warning messages	<input type="checkbox"/> Disable decay of species
<input type="checkbox"/> Log cell-network details	
Source Term	
Barrier failure type:	Random failure time v
<input checked="" type="checkbox"/> Round (vs truncate) the computed number of waste-package failures	
Display Units	
Mass in pathways:	<input type="text" value="g"/> (M)
Mass fluxes:	<input type="text" value="g/yr"/> (M/T)
Fluid concentrations:	<input type="text" value="mg/l"/> (M/L3)
Solid concentrations:	<input type="text" value="g/kg"/> (M/M)
<input type="button" value="Restore defaults"/>	
<input type="button" value="OK"/> <input type="button" value="Cancel"/> <input type="button" value="Help"/>	

## Using External Pathways

External Pathways provide a mechanism by which external program modules for contaminant transport (e.g., analytical, finite element or finite difference solute transport models) can be directly integrated into GoldSim. These modules (referred to as *External pathway functions*) are linked into GoldSim as DLLs (Dynamic Link Libraries) at run time. External pathways are specialized extensions of the External element (discussed in "External (DLL) Elements" in the **GoldSim User's Guide**).

An example file, ExternalPathway.gsm (and the corresponding DLL) can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu). The source code (in C++ and Fortran) for the example can be found in the General Examples/External folder in your GoldSim directory.

### Features and Capabilities of External Pathways

Because your external module is completely defined and created by you, External pathways are extremely flexible. You determine the manner in which the External Pathway operates on the contaminant mass it receives: the External Pathway may be a simple one-dimensional representation, or could be a complex three-dimensional model.

You also define the manner in which the External Pathway is linked to the rest of the GoldSim pathway network by specifying the input mass flux links (i.e., the pathway(s) which discharge mass to the External Pathway) and the output mass flux links (i.e., the pathway(s) to which the External Pathway discharges mass). GoldSim then automatically calls the function representing the External Pathway at the appropriate times, passing the appropriate information back and forth between GoldSim and the function.

Integrating external contaminant transport pathways into GoldSim requires that you develop a "wrapper" (or "shell") around your existing function, and compile it into a DLL. In most cases, this will require only a limited number of programming modifications. GoldSim supports both 32-bit and 64-bit DLLs.



**Warning:** Because GoldSim "loses control" of any species mass that it sends to an External Pathway, it obviously cannot apply solubility and mass balance constraints, and cannot force the reactions defined in the GoldSim model to be applied inside the pathway. Hence, it becomes the responsibility of the author of the function called by the External pathway to do so.

The steps involved in creating and using an External pathway are as follows:

1. Code the function(s) to be used by the External pathway(s) in your model;
2. Compile the functions into a DLL (multiple functions can be included in the same DLL);
3. Create an External pathway element within GoldSim and specify the DLL and the specific function within the DLL to be used;
4. Specify within GoldSim how the External pathway is linked to the pathway network (via mass flux links);
5. Specify any additional input and output arguments that are to be sent to and received from the function.

### **External Pathway Example**

The details of the first two steps are discussed in Appendix C. The other steps are discussed in the following sections.

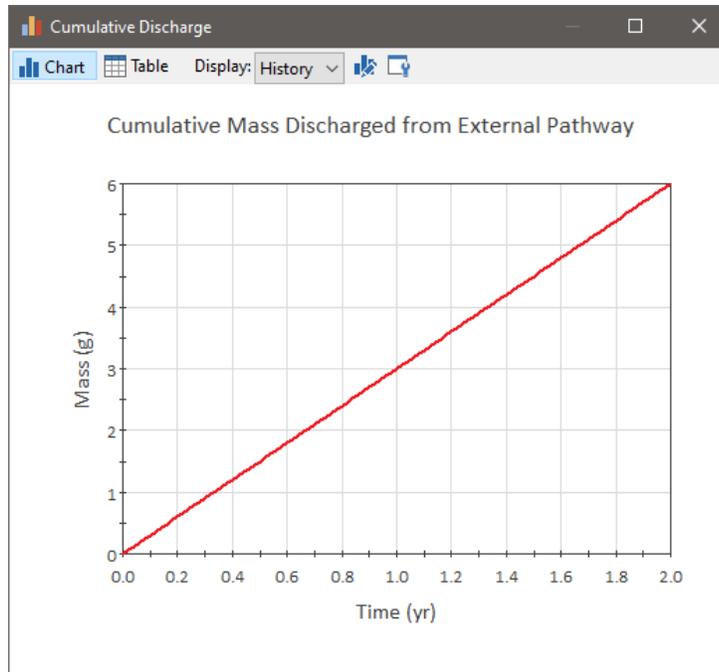
**Read more:** [Appendix C: Implementing External \(DLL\) Pathways](#) (page 385).

Before describing the details involved in using External pathways, let's first examine a very simple example. This particular example file, ExternalPathway.gsm (and the corresponding DLL), can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu). The source code (in C++ and Fortran) for the example can be found in the General Examples/External folder in your GoldSim directory.

In this example, a boundary condition of 1 g/yr is applied to a Cell, which flushes immediately into an External pathway. The External pathway function itself is trivial: in addition to the flux input, it requires an additional dimensionless input. Whenever it is called, it simply multiplies the incoming flux by this value and discharges it. In this particular case, the multiplier is equal to 3. To simulate this system in GoldSim, you would do the following:

1. Code and compile the External pathway function;
2. Define a single species;
3. Define a Cell pathway to represent the source and define its properties (including its boundary condition);
4. Define a single External pathway and define its properties (i.e., the DLL and function it uses);
5. Define a Cell pathway to represent a sink into which the External pathway can discharge;
6. Create advective mass flux links from the source Cell to the External pathway, and from the External pathway to the sink Cell; and
7. Specify the simulation settings (i.e., duration and timestep), and run the model.

The simulation is run for 2 years, so that a total of 2 g of the species enters the system. The output of this simulation, in the form of a time history of the cumulative amount of species mass which is discharged to the sink Cell, is shown below:



Note that mass accumulates at a rate of 3 g/yr (rather than 1 g/yr), since the External pathway multiplies the incoming mass by a factor of 3.

## General Information Flow to and from an External Pathway

Before describing how you specify the properties of an External pathway, it is useful to summarize the general information flow between GoldSim and the External pathway function.

The following information is automatically passed by GoldSim to the External pathway function when it is called:

- any (optional) input arguments that you wish to send to the function (you will always need to pass the current time, but need not send any additional inputs);
- the number of species in the model;
- the number of mass flux links into the pathway;
- the number of mass flux links which GoldSim expects to be returned from the pathway;
- a flag indicating whether all species fluxes in the mass flux links into the pathways are zero for the current call (which you could use to internally instruct the External pathway to skip various calculations); and
- a vector for each mass flux link into the External pathway indicating the quantity of mass of each species passed to the External pathway since the last time it was called (typically one timestep).

GoldSim expects the following information to be returned from the External pathway function when it is called:

- any (optional) output arguments that you wish to return from the function (you need not return any additional outputs);

- a vector for each mass flux link out of the External pathway indicating the quantity of mass of each species passed from the External pathway since the last time it was called (typically one timestep).

The details regarding the manner in which this information is passed is provided in Appendix C.

**Read more:** [Appendix C: Implementing External \(DLL\) Pathways](#) (page 385).

### When is the External Pathway Function Called?

The External pathway function is called at the following times:

- At the beginning of the simulation (Etime = 0);
- Every GoldSim timestep; and
- At any internal (subdivided) timestep in which an Event is triggered (Events and subdivided timesteps are discussed in "Simulating Discrete Events" in the **GoldSim User's Guide**.)

It is likely that you may want to treat each of these calls in a different way. For example, you may wish the External pathway function to ignore the call at the beginning of the simulation, or you may want it to carry out some special initialization routines at that time. You may also want to treat a call in the middle of a timestep (due to an Event) differently from a call at the end of a timestep. In order to communicate this kind of information to the External pathway function, you would need to send **ETime** (the current elapsed time) and perhaps **TimestepLength** (the length of the current timestep) to the External pathway function as optional input arguments.

### Defining External Pathway Properties

The editing dialog for an External pathway is shown below:

The screenshot shows the 'External Pathway Properties' dialog box for 'ExternalPathway1'. It has four tabs: 'Definition', 'Interface', 'Inflows', and 'Outflows'. The 'Definition' tab is selected. The 'Element ID' is 'ExternalPathway1'. There is a 'Description' field. Under 'DLL Options', there is a 'DLL Path' field with a folder icon, a 'Function Name' field, and three checkboxes: 'Lock onto this file', 'Run in separate process', and 'Run Cleanup after each realization'. Below this is the text 'The element defines 0 inputs and 0 outputs.' Under 'Mass Transport Options', there is a 'Mass Units' field with 'g' entered, and two checked checkboxes: 'Combine flux inputs to pathway' and 'Split single flux output from pathway'. There is an 'Initial Inventory' dropdown menu. Under 'Save Non-Flux Results', there are three checkboxes: 'Final Values', 'Time History', and 'Record CPU times in the run log'. At the bottom are 'OK', 'Cancel', and 'Help' buttons.

The sections below describe the various inputs for the External pathway.

### Specifying the External Pathway Function

The primary inputs for an External pathway are the specification of the **DLL** and **Function** which will be used by the External pathway:

**DLL Path:** This is the name of the dynamic link library containing the External pathway function. In general, you must specify the full path to the DLL. (If you specify just the filename, it will look for the DLL only in the working directory containing the GoldSim executable). Note that a single DLL can contain multiple External pathway functions. You can use the Browse button (the folder to the right of the input field) to search for a file.

**Function Name:** This is the specific name of the External pathway function in the DLL. This name is case-sensitive and must exactly match the name of the function in the source code for the External pathway function.

There are also several options that control how the DLL is called by GoldSim:

**Run Cleanup after each realization:** If this box is checked, GoldSim will call the DLL with a cleanup instruction (99) at the end of each realization. (See Appendix C of the **GoldSim User's Guide**.)

**Lock onto this file:** If this box is checked, GoldSim regards various properties of the file (including and alphanumeric code the can be used to determine whether the file contents have changed.

**Read more:** [Locking onto an External Pathway DLL File](#) (page 223).

**Run in separate process:** If this box is checked, GoldSim executes the DLL outside of the GoldSim process space. This can be useful for DLLs that have large memory requirements.

**Read more:** [Running the External Pathway DLL in a Separate Process](#) (page 224).



**Note:** You can use GoldSim's File element to automatically copy the DLL file from some location (typically on a network) to your machine. Because GoldSim records this action in the Run Log, it can provide an "audit trail" to ensure that the proper version of an external file (such as a DLL) was used in a particular simulation. File elements are discussed in detail in the Chapter 10 of the **GoldSim User's Guide**.

---

If you check the **Record CPU times in the run log** box, if the element uses more than 1 CPU seconds, a message will be written to the GoldSim run log identifying the element's name, type (i.e., External Pathway), the number of times it was updated, and the total CPU time used.

GoldSim allows you to "lock onto" the DLL file that is being referenced. When you lock onto a file (by checking the **Lock onto this file** option in the External Pathway element dialog), the following additional information regarding the referenced file is saved with the element:

- File and path name;
- Date the file was created;
- Date the file was last modified;
- File size; and
- CRC signature.

Once you have locked onto a file, this information is displayed in a tool-tip when you hold your cursor over the filename in the dialog.

### **Locking onto an External Pathway DLL File**

The CRC signature is an alphanumeric code that can be used to uniquely identify whether the file contents have changed. When you run a model that has locked onto a file, GoldSim compares the CRC signature of the file with the original signature that was stored. If these are not identical (indicating that the file has been changed), GoldSim displays an error message and will not run the model.

You can unlock a file by clearing the **Lock onto this file** checkbox. Note that if versioning is enabled, whenever a file is locked onto or unlocked, this information is logged with the version.

### Running the External Pathway DLL in a Separate Process

By default, GoldSim loads DLLs used by External elements into the GoldSim process space. GoldSim and the all external DLLs therefore share the application's address space, which is usually limited to 2 GB on Windows operating systems. In some case, a single DLL itself may have large memory requirements (e.g., if it loaded large sets of data from files or databases), or it could statically or dynamically allocate large blocks of memory. If the combined memory requirements of GoldSim (the executable), the GoldSim model (including all model properties, buffers and result values) and all DLLs exceeds 2 GB, GoldSim will be unable to carry out the simulation. The user will be forced to preserve memory by saving fewer histories or timesteps, or by turning off saving of results for certain elements.

To circumvent this limitation, GoldSim provides a feature that allows external DLLs to be executed outside of the GoldSim process space. If **Run in separate process** is checked, GoldSim does not load the DLL into its own process space. Instead, it launches a separate small DLL server with its own private process space. The DLL server works like a middleman who dispatches information between GoldSim and the external DLL. Each DLL that runs in a separate process has its own DLL server. Therefore each DLL has access to a private 2 GB process space, which is not shared with any other DLL or application.



**Note:** 64-bit DLLs *must* be run in a separate process.

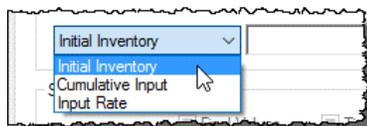
### Defining Initial/Boundary Conditions for an External Pathway

There are two ways by which species mass can enter an External pathway:

- Through a mass flux link from another pathway to the pathway; and/or
- By defining an initial condition and/or a boundary condition (in the form of a cumulative input) for the pathway.

In this section, we discuss defining an initial and/or boundary condition for an External pathway.

An initial condition/boundary condition for an External Pathway is specified using the drop-list toward the bottom of the External Pathway dialog. This drop-list provides three options:



- **Initial Inventory.** This is the default, and represents the initial inventory of each species. This field only accepts vectors by species with dimensions of mass. Moreover, this input cannot be specified as a function of time (if it is, GoldSim will display a fatal error when you try to run the model).

- Cumulative Input.** This option provides a mechanism for simultaneously specifying an initial condition and a rate of mass addition (that may change with time). This field only accepts vectors by species with dimensions of mass. It represents the *cumulative* amount of mass of each species added to the External Pathway at a given time. Hence, if it is constant, it represents an initial condition. If it increases with time, its rate of change represents a specified rate of addition. Correct use of the "Cumulative Input" is summarized in the table below:

To specify this:	Enter the following into the "Cumulative Input" field:
An initial condition	A constant vector with dimensions of mass (in this case, however, it would be more transparent to use the "Initial Inventory" option).
An initial condition and a <i>constant</i> rate of addition	An expression such as: $Initial + Rate * Etime$ , where Initial is a constant vector (with dimensions of mass) and Rate is a constant vector (with dimensions of mass/time).
An initial condition and a <i>time-variable</i> rate of addition	The output of a Pool, Reservoir or Integrator element (with output dimensions of mass) with a specified Initial Value and (time-variable) Rate of Change.



**Warning:** The Cumulative Input must stay constant or increase with elapsed time. That is, you cannot remove mass from an External Pathway using the Cumulative Input field. If the value ever begins to decrease with time, a fatal error occurs.

- Input Rate.** The third option is used to specify a rate of mass addition (that may change with time). This field only accepts vectors by species with dimensions of mass/time. It represents the rate at which mass of each species is added to the Pathway over the next timestep.



**Note:** One way to easily enter a vector of data into an input field without having to create a separate element is to use GoldSim's vector constructor function. For example, entering "vector(1g)" into the Cumulative Input field results in an initial condition of 1 g of each species being present in the Pathway. Vector constructor functions are discussed in detail in "Using Vectors and Matrices" within Chapter 10 of the **GoldSim User's Guide**.



**Note:** GoldSim passes the initial condition/boundary condition to the External pathway function by adding it to the first advective Inflow (or in the absence of Inflows, the first Diffusive Influx) to the External pathway. A separate vector is only sent to the External pathway function if there are no Inflows or Influxes into the pathway.

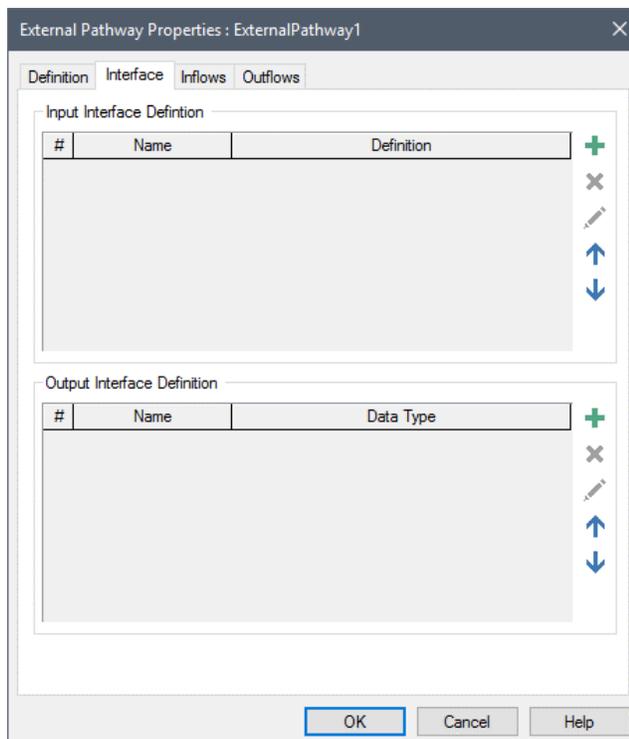
## Adding Input and Output Arguments for an External Pathway

**Read more:** [Flux Links to/from External Pathways](#) (page 228).

In addition to passing the mass flux link data to and from the External pathway function, GoldSim allows you to send and receive additional input and output arguments to and from the function.

This can allow, for example, the External pathway function to utilize the same species properties (e.g., solubilities and partition coefficients) used by other pathways in your model. It also allows you to pass back into your GoldSim model other information that your External pathway function may be computing (e.g., flow rates, heads, total mass in pathway).

You define additional input arguments via the **Interface** tab:



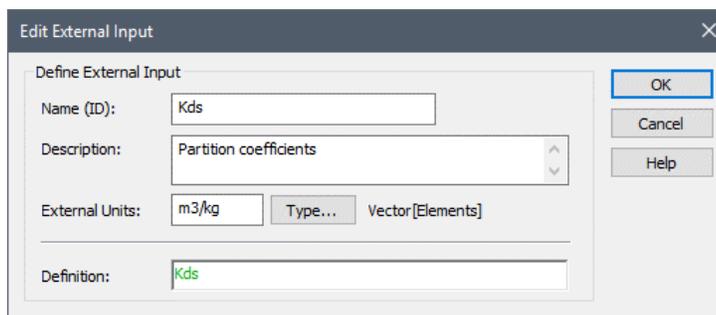
The top part of this dialog is used to define the input arguments. The bottom portion is used to define the output arguments.



Add button

In order to add an input argument, press the Add button in the Input Interface portion of the dialog. When you do this, GoldSim displays the Insert Link dialog, allowing you to select an existing output to add to the interface):

After selecting a link and pressing **OK**, the following dialog is displayed:



The **Definition** displays the output that was selected. The **Name (ID)** defaults to the output name. The **Name (ID)** will appear on the input interface for the External element (accessed via the input port). The **Description** is optional and simply provides additional information regarding the input argument (it defaults to the element description for the output that was selected).

The dimensions of the **External Units** and **Type...** (e.g., value/condition, scalar/vector/matrix) for the input argument are automatically determined by the output that was selected. Prior to sending the argument to the DLL, GoldSim converts it to a number in the **External Units** specified. This can be edited, but must have dimensions consistent with the **Definition**.



**Note:** If you send a output whose **Type** is a Condition to an external function, GoldSim will automatically convert it to either a 0 (for False) or 1 (for True) prior to sending the argument to the DLL.



**Note:** If you pressed **Cancel** (rather than selecting an output) when adding the input argument, the **Definition** (and hence **External Units** and **Type**) will be blank. You could enter any expression into the **Definition** field (including constants). The **External Units** and **Type** would need to be specified in a manner that was consistent with the **Definition**.



Add button

In order to add an output argument, press the Add button in the Output Interface portion of the dialog. When you do this, GoldSim displays the following dialog:

The **Name (ID)** is the name by which the output variable can be referenced in the model. For example, if the name of the External Pathway element was X, and the name of the output was Y, the output could be referenced as X.Y. This ID has the same restrictions as an element ID.

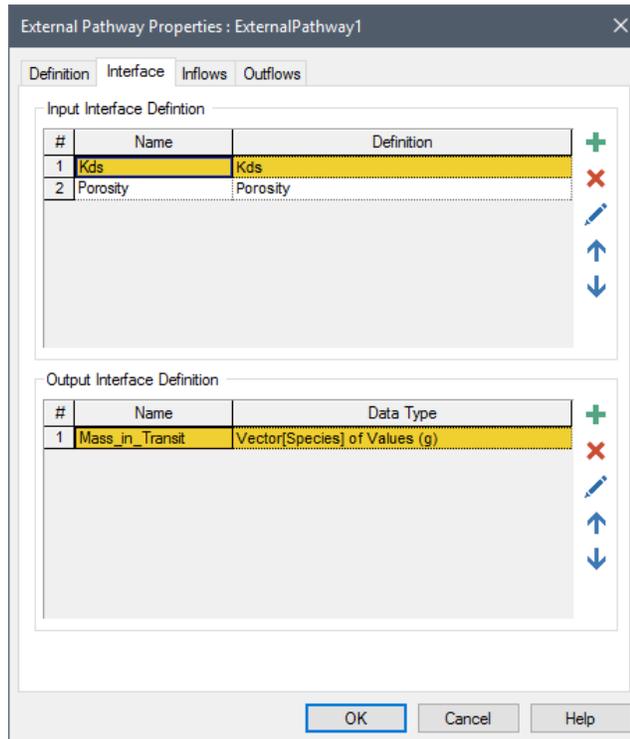
The **Description** is an optional description of the output. The **External Units** represent the units in which the External function returns the value. The specified units also become the Display Units for the output. The **Type...** button is used to access a dialog for specifying the data type (e.g., value/condition, scalar/vector/matrix). (Specifying the order of an output by defining array label sets is discussed in "Using Vectors and Matrices" in the **GoldSim User's Guide**.)



**Note:** If you add an output whose **Type** is a Condition to the output interface, GoldSim will treat any non-zero number as True, and zero as False.

There is no limit to the number of input and output arguments that can be added.

After adding the input and output arguments, the Interface tab displays them as follows:



The input arguments and output arguments are transferred between GoldSim and the external function in exactly the order in which they are listed on the **Interface** tab (inputs first, and then outputs).

Buttons for deleting, editing and moving the input and output arguments up and down in the list are available directly below the Add buttons.

## Flux Links to/from External Pathways

In order to integrate the External pathway into your pathway network, you create mass flux links to and from the pathway.

The only way to transport mass *out* of an External pathway is by specifying an advective mass flux link to another pathway. Diffusive mass flux links *from* External pathways (diffusive outfluxes) and special purpose (direct transfer, precipitate removal and treatment) mass flux links from External pathways cannot be created.

**Read more:** [Understanding Advective Mass Flux Links](#) (page 90).

Note that the flow rate of the fluid defined in an advective mass flux link from a External pathway, if used at all, is only used to determine how mass from a single output vector passed from the External pathway function is apportioned between multiple Outflow flux links

**Read more:** [Passing Mass Flux Data Between GoldSim and the External Pathway Function](#) (page 229).

That is, the mass flux link is used only to specify *where* the mass is to be discharged. The External pathway function itself determines the rate at which mass is discharged to that location.

You can transport mass *into* an External pathway via an advective mass flux link from any other type of pathway and/or via a diffusive mass flux link from a Cell pathway. Within GoldSim, *the concentration and diffusive length on the*

External pathway side of a diffusive mass flux link are assumed to be zero. Hence, like advective mass flux links, diffusive mass flux links involving External pathways are uni-directional.



**Note:** When you create an advective mass flux link from an External pathway, GoldSim will assume that the Reference Fluid is the flowing fluid. Note, however, that because the mass flux link is really only used to determine *where* mass from the External pathway is to be discharged, conceptually the mass flux link can represent any medium (and any type of transport process) you choose. Because all pathways contain a Reference Fluid, you will be able to create an advective mass flux link from an External pathway to any other pathway in the model. Similarly, you can create an advective mass flux link from any pathway in your model to an External pathway, even if the flux link involves a fluid other than the Reference Fluid. That is, unlike advective flux links between other pathway types, GoldSim does not force both pathways to contain the flowing fluid when the link involves an External pathway.

### ***Advection and Diffusion of Particulates into External Pathways***

Suspended solids can advect into an External pathway from other pathways containing suspended solids. Suspended solids can also diffuse into an External pathway from a Cell or Aquifer containing suspended solids. When suspended solids (carrying species mass) enter an External pathway from another pathway, conceptually, the particulates are assumed to immediately disintegrate upon entering the pathway (releasing their species mass to the fluid in the pathway).

**Read more:** [Advection of Particulates to/from Cells](#) (page 138); [Diffusion of Particulates to/from Cells](#) (page 141); [Advection and Diffusion of Particulates to/from Pipes](#) (page 215).

### ***Passing Mass Flux Data Between GoldSim and the External Pathway Function***

Prior to sending the mass flux data to the External pathway function, GoldSim converts the mass flux vectors to mass vectors. These represent the amount of mass (of each species) moving through the link since the last time the External pathway function was called. The External pathway function returns the mass flux data in the same form. GoldSim converts these mass vectors to and from mass fluxes by dividing by the amount of time since the last function call.

The portion of the External pathway dialog labeled "Mass Transport" contains three inputs which control the manner in which mass flux data is passed between GoldSim and the External pathway function:

**Combine flux inputs to pathway:** If this box is checked, GoldSim will combine the mass fluxes for all mass flux links *to* the External pathway into a single vector and pass this to the External pathway function. If the checkbox is cleared, the mass flux links are passed separately to the External pathway function *in the order they are defined* (i.e., the order they are displayed in the **Inflows** tab).

**Split single flux output from pathway:** If this box is checked, GoldSim assumes that a single mass vector will be passed from the External pathway function back to GoldSim. GoldSim then distributes the mass to the specified pathway Outflows in proportion to the specified flow rates for the links. If the checkbox is cleared, GoldSim expects that the External pathway function will pass a separate vector for each specified Outflow *in the order they are defined* (i.e., the order they are displayed in the **Outflows** tab).

**Mass Units:** These are the mass units that the External pathway function expects to receive (and return) mass flux data. GoldSim converts the mass

## External Pathway Outputs

vectors *into* these units prior to sending them to the External pathway function, and converts the returning mass vectors *from* these units (to the internal system units) after receiving them from the function.

External pathways have two types of outputs:

- User-defined output arguments; and
- Mass flux link Outflows.

The user-defined outputs are optional (none need be defined). Their type and dimension are determined by the user when they are created.

For every advective mass flux link in which the External pathway is the Outflow (upstream) pathway, an output is created on the External pathway:

- **Medium\_to\_Path2**, where *Medium* is the name of the flowing medium (which is always the Reference Fluid), and *Path2* is the name of the linked (Inflow) pathway. This is a vector by species, and has dimensions of mass/time. It represents the mass flux of each species from the External pathway to the downstream pathway.

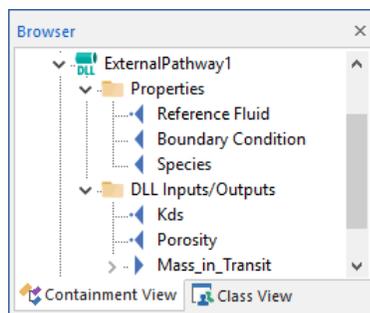
**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94).

It is important to understand that the mass flux outputs from an External Pathway represent the mass rate over the *previous* timestep. This can have implications if you choose to integrate one of these outputs (using an Integrator).

**Read more:** [Manipulating Pathway Outputs](#) (page 253)

## Viewing an External Pathway in the Browser

The browser view of an External pathway is shown below:



The "DLL Inputs/Outputs" folder contains any user-defined input and output arguments.



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

The Properties folder contains the Boundary Condition, Species input, and the Reference Fluid input. The Species input is automatically linked to the nearest Species element when the External pathway is created. Similarly, the Reference Fluid input is automatically linked to the nearest Reference Fluid element when the pathways is created. *These links cannot be changed using the Link Cursor, and are displayed for information purposes only.*

Any mass flux links associated with the External pathway are organized into the Inflows, Outflows, and Diffusive Influxes folders. These folders are not shown if they are empty.

## Saving Results for an External Pathway

**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94); [Inputs and Outputs Associated with Diffusive Mass Flux Links](#) (page 101); [Inputs and Outputs Associated with Direct Transfer Mass Flux Links](#) (page 105); [Inputs and Outputs Associated with Precipitate Removal Mass Flux Links](#) (page 110); [Inputs and Outputs Associated with Treatment Mass Flux Links](#) (page 116).

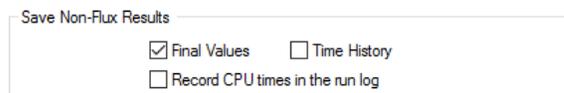
External pathways produce the following outputs:

- value(s) for the user-defined output arguments; and
- the mass flux of each species for all specified advective Outflows.

The types and dimensions of the user-defined outputs are specified by the user when they are created. The flux outputs are vectors by species with dimensions of mass/time.

You specify that you wish to save these results in two different places:

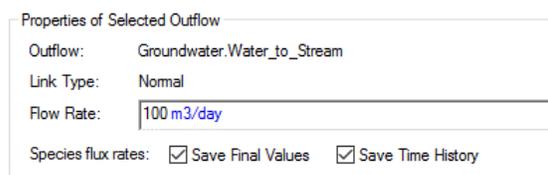
1. All user-defined outputs are saved by clicking **Final Values** and/or **Time History** at the bottom of the External pathway editing dialog:



Checking one of these causes all user-defined output arguments to be saved. If you wish to save only one or two of these as results, you can use the context menu of the output (accessed via a right-click) in the browser to turn on or off a particular output. In this case, the checkbox in the dialog would become gray (indicating that *some* of the results will be saved). The display units for these outputs are defined when the output is created.

As discussed below, if your user-defined outputs are arrays and you are running multiple realizations, time histories are only saved if the output is linked to a Time History Result element.

2. Fluxes are saved by selecting a mass flux link in the Inflows or Outflows tab for a linked pathway and clicking **Save Final Values** and/or **Save Time History** at the bottom of the dialog:

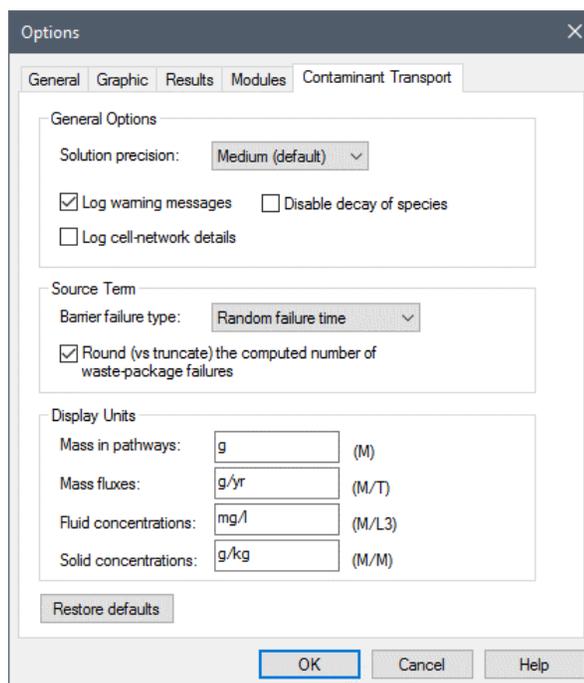


If you are running multiple realizations, the Time History box is ignored, and unless an output of the element is connected to a Time History Result element, no time history results will be saved at all for the element. In fact, in such a case, the Save Results section would look like this:

Final Values     Monte Carlo Histories

In this particular case, because the simulation involves multiple realizations, the “Time History” checkbox is replaced by a “Monte Carlo Histories” checkbox. This checkbox is grayed out, since it is only used for information purposes. You cannot edit it directly, and its appearance is completely determined by whether or not the output is connected to a Time History Result element. That is, in order to save time history results for an External output when running multiple realizations, you must connect it to a Time History Result element.

The display units for masses, concentrations and fluxes for all pathways are specified in the **Contaminant Transport** tab of the Options dialog (accessed via **Model | Options...** from the main menu):



## Using Network Pathways

Network Pathways use a Laplace-transform approach to provide a computationally efficient way to simulate large, complex networks of one-dimensional conduits in order to describe contaminant transport through fractured rock systems. Network pathways are only available within the RT Module.

### Features and Capabilities of Network Pathways

A Network Pathway is made up of multiple “pipes”. The fact that these are referred to as pipes is not coincidental - each fracture network pipe has all the features and capabilities of the Pipe pathways discussed previously. In fact, Network pathways are effectively large collections of Pipe pathways. Like Pipe pathways, Network pathways contain only a single fluid medium (which is always, by definition, the Reference Fluid).

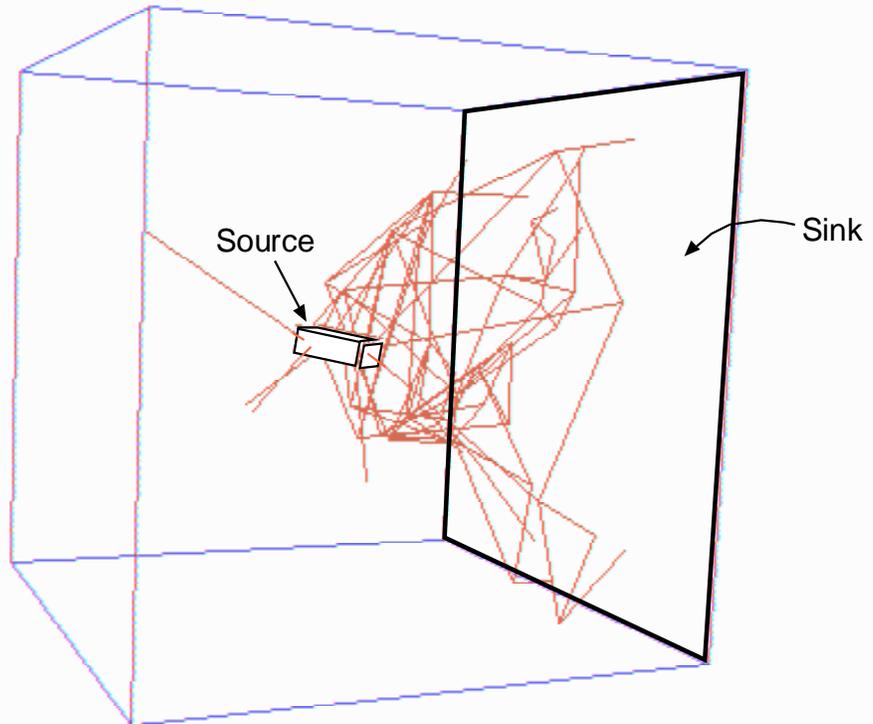
Network Pathways require specification of a *fracture network*, which can be entered by hand, but more likely would be generated by a discrete fracture network generation and flow simulation code. The fracture network identifies all of the pipes in the network, the manner in which they are connected, and each pipe's geometry and flow rate.

In addition, for each pipe in the fracture network, a *fracture set* is specified, which identifies the transport properties of the pipe (e.g., porous infill material, coating material, properties of matrix diffusion zones, etc.). The network of pipes can be very large (e.g., 100,000 pipes). This allows complex and realistic fracture systems to be simulated.



**Warning:** Solubility constraints are not applied within Network pathways. (They are only applied within Cells and Aquifers). Hence, if the concentration of a species entering a Network pathway (e.g., via a boundary condition) exceeded the solubility limit, the concentration leaving the Network could exceed the solubility limit.

A schematic of a relatively small three-dimensional fracture network that could be simulated by GoldSim is shown below:



In addition to defining the fracture network, it is necessary to identify the mass flux links to and from the Network pathway (referred to as "sources" and "sinks", respectively), and specify the properties for all of the fracture sets referenced by the fracture network. Although there may be a very large number of "pipes" (100,000 or more), it is assumed that these can all be grouped into a relatively small (typically ten or less) number of fracture sets.

To facilitate representation of uncertainty in the fracture network connectivity and flow properties, you have the option to define a number of separate fracture networks and instruct GoldSim to randomly select one of these every realization.

The ability to solve Network pathways efficiently results from the fact that it is possible to develop a Laplace-transformed transfer matrix for an entire network of Pipe pathways by simple additions and multiplications of the transformed transfer matrices for each individual pathway. Once the network transfer matrix/matrices are developed, then the transport calculations for the network are no more time-consuming than for a single Pipe pathway. The only extra computational expense is the time required for the creation of the network transfer matrix at the beginning of the simulation. For even quite large networks (100,000 pipes or more), this time is not excessive.

The mathematical details of Network pathways are discussed in Appendix B. The following sections describe the basic assumptions incorporated into Network pathways, and how to define and use them in your models.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

## Defining Network Pathway Properties

The editing dialog for a Network pathway is shown below:

The sections below describe the various input for the Network pathway.

### What is a Fracture Network?

The primary input to a network pathway is the *fracture network*. Each Network pathway requires at least one fracture network. Very simple fracture networks can be entered by hand, but complex fracture networks would typically be generated by a discrete fracture network generation and flow simulation code. (Golder Associates' FracMan library of codes for fractured-rock systems includes a program, called PAWorks, which can generate fracture network files that can be directly imported into GoldSim).

This fracture network identifies all of the “pipes” making up the pathway, and the manner in which they are interconnected. In addition, for each pipe, it identifies:

- the geometry (length, cross-sectional area, and flow-wetted area);
- the flow rate; and
- the *fracture set*, which identifies the transport properties of the pipe (e.g., porous infill material, coating material, properties of matrix diffusion zones, etc.).

Finally, the fracture network identifies which of the pipes are associated with "sources" (mass flux links into the pathway) and which pipes are associated with "sinks" (mass flux links out of the pathway) and/or "watch groups" (collections of pipes within the network whose mass fluxes can be added together and monitored).

## Creating and Editing the Fracture Network

A fracture network can be created or edited by pressing the **Edit Fracture Network...** button, which will display the following dialog:

Pipe	Length [m]	Flow [m3/yr]	Area [m2]	Awet [m2]	Properties	Source	Sink	Upstream Paths
1	20	0.819173	0.00964563	610	SET_1		Watch01	2
2	20	0.879867	0.0127828	808.4	SET_1		Watch02	3
3	20	1.30806	0.017457	1104	SET_1		Watch03	16
4	20	1.73638	0.017888	800	SET_1		Watch04	6, 18, 19
5	20	2.85418	0.0238569	1058	SET_1		Watch05	4, 20, 22
6	20	1.19785	0.0121191	542	SET_1		Watch06	14
7	20	3.44909	0.0253	800	SET_1		Watch07	9
8	20	3.00444	0.0171407	542	SET_1		Watch08	7, 21
9	20	3.89948	0.0305751	966.8	SET_1		Watch09	13
10	20	7.30741	0.0381773	853.6	SET_2		Watch10	11, 17
11	20	6.96732	0.0404672	904.8	SET_2		Watch11	15
12	20	6.69494	0.0250818	560.8	SET_2		Watch12	10
13	20	10.8668	0.14176	708.8	SET_2		Watch13	14
14	20	12.0651	0.1808	904	SET_2		Watch14	16
15	20	6.9672	0.18144	907.2	SET_2		Watch15	13
16	20	13.3724	0.29856	1492.8	SET_2	BG1	Watch16	3, 14
17	20	0.339656	0.19288	964.4	SET_1		Watch17	9
18	20	0.11009	0.16	800	SET_1		Watch18	9
19	20	0.428057	0.1484	742	SET_1		Watch19	3
20	20	1.05681	0.16	800	SET_1		Watch20	7, 21
21	20	0.61247	0.13784	689.2	SET_1		Watch21	10
22	20	0.0607056	0.17328	866.4	SET_1		Watch22	2
23	20	6.67778	0.08272	413.6	SET_2		Watch23	8, 24
24	20	3.67335	0.16	800	SET_2		Watch24	5, 26
25	20	13.3727	0.1224	612	SET_2	BG2; Watc	12, 23	23
26	20	0.819207	0.16032	801.6	SET_2		Watch26	1

This dialog contains 10 columns. Each row represents a different pipe in the network. A predefined network of pipes can be read from a separate text file by pressing the **Import...** button. The format for this file is described in Appendix D.

**Read more:** [Appendix D: Network Pathway File Format](#) (page 393).

Pipes can be added (to the end of the list) and deleted manually using the **Add Pipe** and **Delete Pipe** buttons. Each column (except the first) can be edited by the user. *None of the fields, however, accept links or units. In fact, unlike any other input dialogs in GoldSim, when defining a fracture set, the units for the inputs are predefined.* The ten columns are described below:

**Pipe:** This is the pipe number. Pipes are numbered sequentially, and therefore this field cannot be edited.

**Length:** This is the length of the pipe, *in meters*.

**Flow:** This is the total flow rate in the pipe, *in cubic meters per year*.

**Area:** This is the cross-sectional area of the pipe, *in square meters*.

**Awet:** This is the wetted area of the pipe (wetted perimeter multiplied by length), *in square meters*.

**Properties:** This is the name of the fracture set for the pipe. Fracture Sets define the transport properties for the pipe. As such, it must be the name of an existing Fracture Set element in the model.

**Read more:** [Defining Fracture Sets](#) (page 241).

**Source:** This field, which can be empty, contains the name of a "source" which is linked to the pipe. As such, it must be the name of an existing pathway in the model which has a mass flux link *into* the Network pathway.

**Sink:** This field, which can be empty, contains the name of a "sink" which is linked to the pipe. As such, it must be the name of an existing pathway in the model which has an inflowing mass flux link *from* the Network pathway.

**Read more:** [Defining Sources and Sinks for the Fracture Network](#) (page 236).



**Note:** The Sink field can also contain the name of one or more "watch groups" (separated by semicolons). Each watch group has the form WatchNNN, where NNN is a number between 1 and 999.

---

**Read more:** [Defining Watch Groups for the Fracture Network](#) (page 237).

**Upstream Paths:** This field helps to define the manner in which the pipe is interconnected with the other pipes. It lists the numbers (separated by commas) of all pipes which are immediately *upstream* of the current pipe.

**Downstream Paths:** This field helps to define the manner in which the pipe is interconnected with the other pipes. It lists the numbers (separated by commas) of all pipes which are immediately *downstream* of the current pipe.

---



**Note:** If the file contains more than 1000 pipes, although all pipes will be loaded into the model, only the first 1000 will be displayed in this dialog. In this case, in order to edit any of the pipes (including those that are displayed), you must directly edit the file. That is, the dialog displays the first 1000 pipes, but does not allow you to edit them.

---

### **Defining Sources and Sinks for the Fracture Network**

Each fracture set must have at least one *source* and at least one *sink*. Sources and sinks identify how incoming mass flux links and outgoing mass flux links are mapped to specific locations (pipes) in the Network pathway.

A source is a linked pathway (or boundary condition) which discharges mass *to* one or more pipes in the network. A sink is a linked pathway to which mass is discharged *from* one or more pipes in the network. As a result, any entry in the Source column of the Fracture Network editing dialog must be the name of an existing pathway with a mass flux link that discharges mass to the Network pathway (i.e., is an Outflow or Outflux pathway). Similarly, any entry in the Sink column of the Fracture Network editing dialog must be the name of an existing pathway with a mass flux link that receives mass from the Network pathway (i.e., is an Inflow pathway).

---



**Note:** There are two circumstances in which the entries in the Source column need not be existing pathway names: when combining flux inputs, and when defining initial and boundary conditions.



**Note:** There are two circumstances in which the entries in the Sink column need not be existing pathway names: when splitting flux outputs, and when using Watch Groups.

---

**Read more:** [Combining and Splitting Fluxes to Create Single Sources and Sinks](#) (page 239); [Defining Initial/Boundary Conditions for a Network Pathway](#) (page 239); [Defining Watch Groups for the Fracture Network](#) (page 237).

Multiple pipes can be associated with a particular source or sink. If the fracture network assigns multiple pipes to a source (i.e., if the same pathway is listed in the Source column for multiple pipes), GoldSim allocates the incoming flux from the source pathway to the pipes in proportion to their flow rates. If the fracture network assigns multiple pipes to a sink (i.e., if the same pathway is listed in the Sink column for multiple pipes), GoldSim collects the outgoing fluxes from these pipes and discharges them to the sink pathway.

**Read more:** [Flux Links to/from Network Pathways](#) (page 244).

Note that the fracture network does not have to terminate at the sources and sinks. A source or sink can be thought of as a "window" within the fracture network where species masses are injected or withdrawn.

### Defining Watch Groups for the Fracture Network

Watch Groups are groups of pipes for which the total mass through-flux will be output. Each Watch Group can be thought of as a window within the network, with the rate of flux through the window being provided as an output.

The purpose of Watch Groups is to allow the analyst to view the movement of contaminant masses across internal boundaries in the network, such as the interfaces between geological strata or fault zones.

In order to enable Watch Groups, you must first select the **Number of Watch Groups** you wish to define in the main Network pathway dialog:

Mass Transport

Cumulative Input

Combine flux inputs to pathway

Split single flux output from pathway

Number of Watch Groups: 99

You can define up to 999 Watch Groups.

You must then assign pipes in the network to Watch Groups. There are two ways to do this.

The first method to assign pipes to Watch Groups is via the "Sink" column in the Fracture Network definition dialog (accessed via the **Edit Fracture Network...** button):

Pipe	Length [m]	Flow [m3/yr]	Area [m2]	Awet [m2]	Properties	Source	Sink	Upstream Paths
1	20	0.819173	0.00964563	610	SET_1		Watch01	26
2	20	0.879967	0.0127828	808.4	SET_1		Watch02	3, 1, 22
3	20	1.30806	0.017457	1104	SET_1		Watch03	16
4	20	1.73638	0.017888	800	SET_1		Watch04	6, 18, 19
5	20	2.85418	0.0236569	1058	SET_1		Watch05	4, 20, 22
6	20	1.19785	0.0121191	542	SET_1		Watch06	14
7	20	3.44909	0.0253	800	SET_1		Watch07	9, 8, 20
8	20	3.00444	0.0171407	542	SET_1		Watch08	7, 21
9	20	3.89948	0.0305751	966.8	SET_1		Watch09	13, 7, 17,
10	20	7.30741	0.0381773	853.6	SET_2		Watch10	11, 17
11	20	6.96732	0.0404672	904.8	SET_2		Watch11	15
12	20	6.69494	0.0250818	560.8	SET_2		Watch12	10
13	20	10.8668	0.14176	708.8	SET_2		Watch13	14
14	20	12.0651	0.1808	904	SET_2		Watch14	16
15	20	6.9672	0.18144	907.2	SET_2		Watch15	13
16	20	13.3724	0.29856	1492.8	SET_2	BG1	Watch16	3, 14
17	20	0.339656	0.19288	964.4	SET_1		Watch17	9
18	20	0.11009	0.16	800	SET_1		Watch18	9
19	20	0.428057	0.1484	742	SET_1		Watch19	3
20	20	1.05681	0.16	800	SET_1		Watch20	7, 21
21	20	0.61247	0.13784	689.2	SET_1		Watch21	10
22	20	0.0607056	0.17328	866.4	SET_1		Watch22	2
23	20	6.67778	0.08272	413.6	SET_2		Watch23	8, 24
24	20	3.67335	0.16	800	SET_2		Watch24	5, 26
25	20	13.3727	0.1224	612	SET_2	BG2; Wate	Watch25	12, 23
26	20	0.819207	0.16032	801.6	SET_2		Watch26	1

You assign a pipe to a Watch Group by entering a string *WatchNNN* into the "Sink" column, where NNN is a number between 001 and 999. NNN cannot exceed the number of Watch Groups you have defined. You can enter single digit numbers using a preceding zero, but this is optional (*Watch1*, *Watch01* and *Watch001* are all valid strings).

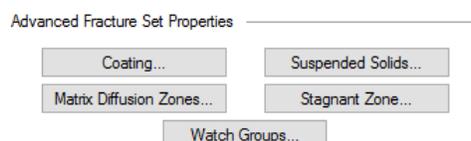


**Note:** You assign multiple Watch Groups and/or a Watch Group and a Sink to a pipe by separating the names with semicolons.

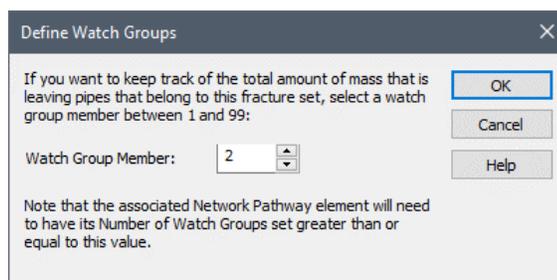
The second method to assign pipes to Watch Groups is via the Fracture Set definition. Each pipe in a fracture network has a Fracture Set assigned to it.

**Read more:** [Defining Fracture Sets](#) (page 241).

The Fracture Set dialog provides an option to assign a Watch Group to the Fracture Set:



Pressing the **Watch Groups...** button in the Fracture Set dialog displays the following dialog allowing you to assign a Watch Group to the Fracture Set:



When this is done, GoldSim will add the discharges from all pipes that are members of this Fracture Set *and* that either discharge to pipes that are not members of the Fracture Set or discharge to unspecified downstream pipes (i.e., no downstream pipe is defined).

For each Watch Group, GoldSim adds an output to the Network pathway (a vector of species with dimensions of mass/time) that represents the discharge from the Watch Group.

**Read more:** [Network Pathway Outputs](#) (page 243).

### Checking the Flow Balance in a Fracture Network

To ensure that the fracture network that you have specified balances flows in an appropriate manner, GoldSim writes a warning message to the Run Log under the following conditions:

- A flowing pipe has no downstream pipe (or sink) to discharge to, and its flow exceeds 1% of the total flow through the sources.
- An upstream pipe (or group of pipes) has more flow than the downstream pipe (or group of pipes) by an amount exceeding 1% of the total flow through the sources, and the upstream/downstream discrepancy exceeds 1% of the flow in the downstream pipe (or group of pipes).

## Combining and Splitting Fluxes to Create Single Sources and Sinks

The portion of the Network pathway dialog labeled "Mass Transport" contains two inputs which control the manner in which mass fluxes are mapped to pipes in the Network pathway:

**Combine flux inputs to pathway:** If this box is checked, GoldSim will combine the mass fluxes for all mass flux links *to* the Network pathway into a single vector. GoldSim allocates the incoming flux vector to the Source pipes in the fracture network in proportion to their flow rates. (In this situation, the source names need not correspond to existing pathways, as the name is used only to identify the pipe as a source, not to direct the incoming mass).

If the checkbox is cleared, the mass flux links are passed separately to the Network pathway and each entry in the Source column must be an existing pathway with a mass flux link that discharges mass to the Network pathway (or "-source-" to indicate an initial/boundary condition, if there are no mass flux links).

**Read more:** [Defining Initial/Boundary Conditions for a Network Pathway](#) (page 239).

**Split single flux output from pathway:** If this box is checked, GoldSim creates a single mass vector by summing all of the fluxes from Sink pipes, and then distributes the mass to the specified Outflow pathways in proportion to the specified flow rates for the links. (In this situation, the sink names need not correspond to existing pathways, as the name is used only to identify the pipe as a sink, not to direct the outgoing mass).

If the checkbox is cleared, GoldSim expects that the Network pathway will pass a separate vector for each specified Outflow, and any entry in the Sink column of the Fracture Network editing dialog must be an existing pathway with a mass flux link that receives mass from the Network pathway.

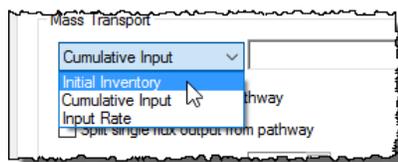
## Defining Initial/Boundary Conditions for a Network Pathway

There are two ways by which species mass can enter a Network pathway:

1. Through a mass flux link from another pathway to the Network pathway; and/or
2. By defining an initial condition and/or a boundary condition (in the form of a cumulative input) for the Network pathway.

In this section, we discuss defining an initial and/or boundary condition for a Network pathway.

An initial condition/boundary condition for a Network Pathway is specified using the drop-list in the "Mass Transport" section of the dialog. This drop-list provides three options:



- **Initial Inventory.** This is the default, and represents the initial inventory of each species. This field only accepts vectors by species with dimensions of mass. Moreover, this input cannot be specified as a function of time (if it is, GoldSim will display a fatal error when you try to run the model).
- **Cumulative Input.** This option provides a mechanism for simultaneously specifying an initial condition and a rate of mass

addition (that may change with time). This field only accepts vectors by species with dimensions of mass. It represents the *cumulative* amount of mass of each species added to the Network Pathway at a given time. Hence, if it is constant, it represents an initial condition. If it increases with time, its rate of change represents a specified rate of addition. Correct use of the "Cumulative Input" is summarized in the table below:

To specify this:	Enter the following into the "Cumulative Input" field:
An initial condition	A constant vector with dimensions of mass (in this case, however, it would be more transparent to use the "Initial Inventory" option).
An initial condition and a <i>constant</i> rate of addition	An expression such as: $Initial + Rate * Etime$ , where Initial is a constant vector (with dimensions of mass) and Rate is a constant vector (with dimensions of mass/time).
An initial condition and a <i>time-variable</i> rate of addition	The output of a Pool, Reservoir or Integrator element (with output dimensions of mass) with a specified Initial Value and (time-variable) Rate of Change.



**Warning:** The Cumulative Input must stay constant or increase with elapsed time. That is, you cannot remove mass from a Network Pathway using the Cumulative Input field. If the value ever begins to decrease with time, a fatal error occurs.

- **Input Rate.** The third option is used to specify a rate of mass addition (that may change with time). This field only accepts vectors by species with dimensions of mass/time. It represents the rate at which mass of each species is added to the Pathway over the next timestep.



**Note:** One way to easily enter a vector of data into an input field without having to create a separate element is to use GoldSim's vector constructor function. For example, entering "vector(1g)" into the Cumulative Input field results in an initial condition of 1 g of each species being present in the Pathway. Vector constructor functions are discussed in detail in "Using Vectors and Matrices" within Chapter 10 of the **GoldSim User's Guide**.

GoldSim passes the initial condition/boundary condition to the Network pathway function by adding it to the first advective Inflow (or in the absence of Inflows, the first Diffusive Influx) to the Network pathway. If you do not have any incoming mass flux links (or if "Combine flux inputs" is checked), the initial and boundary conditions will be distributed over all pipes with Sources defined.



**Note:** If you do not have any incoming flux links, the source pipes must be identified in the fracture network by using the name “-source-” in the Source column.

**Read more:** [Flux Links to/from Network Pathways](#) (page 244).

## Randomly Sampling Fracture Network Files

The Fracture Network dialog allows you to define multiple fracture networks:

Pipe	Length [m]	Flow [m3/yr]	Area [m2]	Awet [m2]	Properties	Source	Sink	Upstream Paths
1	20	0.819173	0.00964563	610	SET_1		Watch01	2
2	20	0.879867	0.0127828	808.4	SET_1		Watch02	3
3	20	1.30806	0.017457	1104	SET_1		Watch03	16
4	20	1.73638	0.017888	800	SET_1		Watch04	6, 18, 19
5	20	2.85418	0.0236569	1058	SET_1		Watch05	4, 20, 22
6	20	1.19785	0.0121191	542	SET_1		Watch06	14
7	20	3.44909	0.0253	800	SET_1		Watch07	9
8	20	3.00444	0.0171407	542	SET_1		Watch08	7, 21
9	20	3.89948	0.0305751	966.8	SET_1		Watch09	13
10	20	7.30741	0.0381773	853.6	SET_2		Watch10	11, 17
11	20	6.96732	0.0404672	904.8	SET_2		Watch11	15
12	20	6.69494	0.0250818	560.8	SET_2		Watch12	10
13	20	10.8668	0.14176	708.8	SET_2		Watch13	14
14	20	12.0651	0.1808	904	SET_2		Watch14	16
15	20	6.9672	0.18144	907.2	SET_2		Watch15	13
16	20	13.3724	0.29856	1492.8	SET_2	BG1	Watch16	3, 14
17	20	0.339656	0.19288	964.4	SET_1		Watch17	9
18	20	0.11009	0.16	800	SET_1		Watch18	9
19	20	0.428057	0.1484	742	SET_1		Watch19	3
20	20	1.05681	0.16	800	SET_1		Watch20	7, 21
21	20	0.61247	0.13784	689.2	SET_1		Watch21	10
22	20	0.0607056	0.17328	866.4	SET_1		Watch22	2
23	20	6.67778	0.08272	413.6	SET_2		Watch23	8, 24
24	20	3.67335	0.16	800	SET_2		Watch24	5, 26
25	20	13.3727	0.1224	612	SET_2		BG2; Watc	12, 23
26	20	0.819207	0.16032	801.6	SET_2		Watch26	1

The current fracture network number being viewed, and the total number of fracture networks defined, are listed at the top of the dialog (“Network X of Y”). You can add and delete new fracture networks using the **Add Network** and **Delete Network** buttons. The **Previous** and **Next** buttons allow you to move between the existing fracture networks that you have defined.

If you define multiple fracture networks, you can tell GoldSim to randomly sample one of them each realization by specifying a **Random variable to select fracture network** in the main Network pathway dialog. If you specify a single fracture network, this input is ignored. Otherwise, this value is used to select the fracture network that is used for a particular realization. In particular, the value is rounded up to the nearest integer, and that integer identifies the fracture set to use for the realization. For example, if you defined three fracture sets, defining the **Random variable to select fracture network** as a uniform distribution between 0 and 3 would result, on average, in all three fracture networks having an equal probability of occurrence. If you had defined multiple fracture networks, but wished to run a simulation in which only a particular one was used, you would simply enter the number of that fracture set (as a constant).



**Warning:** If **Random variable to select fracture network** is entered (or realized) as a number which is invalid (i.e., negative or greater than the number of fracture networks), GoldSim will use the first fracture network.

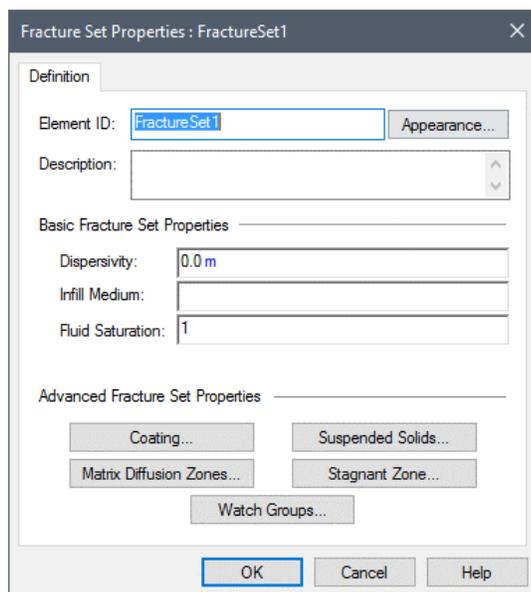
## Defining Fracture Sets

Each pipe in a fracture network has an assigned fracture set. Fracture sets define the transport properties for the pipe. Although there may be a very large number of “pipes” (100,000 or more) in a fracture network, it is assumed that these can

all be grouped into a relatively small (typically ten or less) number of fracture sets.

Fracture set properties are defined using a Fracture Set element. Each fracture set name in the fracture network must correspond to an existing Fracture Set element in your model.

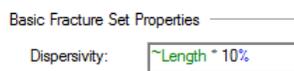
The Fracture Set dialog is shown below:



Note that the Fracture Set dialog is simply a subset of the Pipe dialog. The basic Fracture Set properties are identical to the basic Pipe pathway properties.

**Read more:** [Other Basic Pipe Properties](#) (page 199).

Note that the **Dispersivity** input field supports the Locally available property called "~Length":



When defining the dispersivity for a pipe that references the fracture set, "~Length" is interpreted by GoldSim to be the length of the pipe. This provides a mechanism to make the dispersivity a function of the pipe length (as shown above).



**Note:** Locally available properties are special attributes and are similar to element outputs. However, they are only visible via the Insert Link browser within the fields in which they can be referenced (in this case, the **Dispersivity** field). Locally available properties derive their name from the fact that they may only be available, or they may take on different values (i.e., be over-ridden), in “local” parts of your model (e.g., within a particular element, or within a particular input field for an element). Locally available properties are discussed in detail in Chapter 10 of the **GoldSim User's Guide**.

The advanced Fracture Set properties are also analogous to those specified for a Pipe pathway:

**Coating...** accesses a dialog for defining a sorptive coating material.

**Read more:** [Defining a Sorptive Coating Material for a Pipe](#) (page 205).

**Matrix Diffusion Zones...** accesses a dialog for defining matrix diffusion zones.

**Read more:** [Defining Matrix Diffusion Zones](#) (page 208).

**Stagnant Zone...** accesses a dialog for defining a stagnant dispersive zone.

**Read more:** [Defining a Stagnant Dispersive Zone](#) (page 211).

**Suspended Solids...** accesses a dialog for specifying suspended Solids in the pipe.

**Read more:** [Simulating Suspended Solids in a Pipe](#) (page 212).

The Fracture Set dialog contains one additional button (that is not contained in Pipe dialogs). The **Watch Groups...** button is used to assign a Watch Group to a Fracture Set.

**Read more:** [Defining Watch Groups for the Fracture Network](#) (page 237).

## Network Pathway Outputs

Network pathways have at least two outputs:

- **Mass\_in\_Pathway.** This is a vector by species with dimensions of mass. It represents the total mass of each species in the Network pathway.
- **Concentration.** This is a vector by species with dimensions of mass per volume. It represents the average concentration of each species in the Reference Fluid at the point(s) that it exits the Network pathway (i.e., it is computed as the total mass outflux divided by the total Reference Fluid flow rate).

For every advective mass flux link in which the Network pathway is the Outflow (upstream) pathway, an output is created on the pathway:

- **Medium\_to\_Path2,** where *Medium* is the name of the flowing medium, and *Path2* is the name of the linked (Inflow) pathway. This is a vector by species, and has dimensions of mass/time. It represents the mass flux of each species from the Network pathway to the downstream pathway.

**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94).

It is important to understand that the mass flux outputs from a Network Pathway represent the mass rate over the *previous* timestep. This can have implications if you choose to integrate one of these outputs (using an Integrator).

**Read more:** [Manipulating Pathway Outputs](#) (page 253)

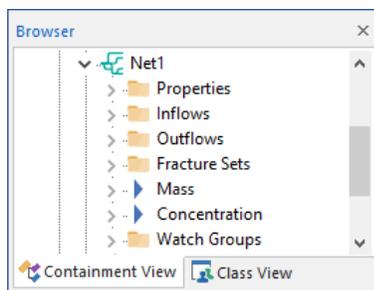
For every Watch Group defined for the pathway, an output is created on the pathway:

- **Watch $_{NN}$ ,** where  $_{NN}$  is the Watch Group number. This is a vector by species, and has dimensions of mass/time. It represents the mass flux of each species from the Watch Group.

**Read more:** [Defining Watch Groups for the Fracture Network](#) (page 237).

## Viewing a Network Pathway in the Browser

The browser view of a Network pathway is shown below:



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

The pathway's mass and concentration outputs are listed first. Note that for a Network pathway, the concentration always refers to the Reference Fluid.

The Properties folder contains the Species input and the Reference Fluid input. The Species input is automatically linked to the nearest Species element when the Network pathway is created. Similarly, the Reference Fluid input is automatically linked to the nearest Reference Fluid element when the pathway is created. *These links cannot be changed using the Link Cursor, and are displayed for information purposes only.* The Properties folder also includes the Boundary Condition for the pathway and the Random variable used to select the fracture network.

Any fracture sets referenced by the fracture network(s) are contained in the Fracture Sets folder.

Any Watch Group outputs are organized into a Watch Group folder.

Any mass flux links associated with the Network pathway are organized into the Inflows, Outflows, and Diffusive Influxes folders.

**Read more:** [Inputs and Outputs Associated with Advective Mass Flux Links](#) (page 94); [Inputs and Outputs Associated with Diffusive Mass Flux Links](#) (page 101); [Inputs and Outputs Associated with Direct Transfer Mass Flux Links](#) (page 105); [Inputs and Outputs Associated with Precipitate Removal Mass Flux Links](#) (page 110); [Inputs and Outputs Associated with Treatment Mass Flux Links](#) (page 116).

## Flux Links to/from Network Pathways

The only way to transport mass *out* of a Network pathway is by specifying an advective mass flux link to another pathway. For Network pathways, the flowing medium is always the Reference Fluid. Diffusive mass flux links *from* Network pathways (diffusive outfluxes) and special purpose (direct transfer, precipitate removal and treatment) mass flux links *from* Network pathways cannot be created.

**Read more:** [Understanding Advective Mass Flux Links](#) (page 90).

Note that *the flow rate of the fluid defined in an advective mass flux link from a Network pathway, if used at all, is only used to determine how mass from a single sink is apportioned between Outflow flux links.*

**Read more:** [Combining and Splitting Fluxes to Create Single Sources and Sinks](#) (page 239).

That is, the mass flux link is used only to specify *where* the mass is to be discharged. The pipe flow rates within the fracture network determine how

mass moves through the pathway and the rate at which mass is discharged. Because the flow rates in the mass flux links to/from Network pathways do not impact the manner in which mass is transported, GoldSim does not test to ensure that the flows in the flux links to and from the pathway are consistent with the internal flows in the network pipes.

You can transport mass *into* a Network pathway via an advective mass flux link from any other type of pathway and/or via a diffusive mass flux link from a Cell pathway. Within GoldSim, *the concentration and diffusive length on the Network pathway side of a diffusive mass flux link are assumed to be zero.* Hence, like advective mass flux links, diffusive mass flux links involving Network pathways are uni-directional.



**Warning:** GoldSim does not enforce a balance for the flow of the Reference Fluid in a Network pathway. That is, the Inflows into the pathway do not need to be equal to the Outflows from the pathway. Unlike Cells and Pipes, however, if the specified Outflows are less than the specified Inflows, it does not imply that the species concentrations leaving the Network pathway would be greater than those entering the pathway. This is because not all of the mass that enters a Network pathway necessarily must exit the pathway, since you may choose to ignore some sinks (e.g., those that discharge to deep locations and effectively leave the system).

---

**Read more:** [Mass Balance in a Network Pathway](#) (page 246); [Checking the Flow Balance in a Fracture Network](#) (page 238).

### **Advection and Diffusion of Particulates to/from Network Pathways**

Suspended solids can advect and diffuse into Network pathways, and can advect out of Network pathways. The advection of suspended solids within pipes in fracture networks is identical to the behavior of suspended solids within Pipe pathways.

**Read more:** [Simulating Suspended Solids in a Pipe](#) (page 212).

Suspended solids can advect into a Network pathway from other pathways containing suspended solids. Suspended solids can also diffuse into a Network pathway from a Cell or Aquifer containing suspended solids. The species mass associated with the suspended solids in the upstream (Outflow or Outflux) pathway enter the Network pathway regardless of whether suspended solids are specified as being present in the pathway. When suspended solids (carrying species mass) enter a Network pathway from another pathway, conceptually, the particulates are assumed to immediately disintegrate upon entering the pathway (releasing their species mass to dissolve in the fluid in the pathway). If suspended solids are present in pipes in the Network pathway, the species mass will then partition onto these solids.

---



**Note:** GoldSim uses the advective and diffusive flux of particulates only to transport species mass and does not keep track of the movement of the suspended Solid media through the pathway network. That is, the flux of particulates has no affect on the quantity of the suspended Solid present in either the Outflux or Influx pathway.

---

**Read more:** [Advection of Particulates to/from Cells](#) (page 138); [Diffusion of Particulates to/from Cells](#) (page 141).

## Mass Balance in a Network Pathway

Not all of the mass of a non-decaying species that enters the pathway necessarily has to exit the pathway. This is because when creating the fracture network, not all of the locations where flow is discharged from the system need to be identified as sinks. Mass that exits the system elsewhere is effectively "lost" and will never re-enter other GoldSim pathways. Note, however, that when GoldSim reports the total mass in the pathway, it includes this "lost" mass.

If you do not wish to "lose" any mass in a Network pathway, all discharge locations for the fracture network must be specifically mapped sinks.

## Controlling the Network Pathway Solution Algorithm

Because Network pathways are based on the same Laplace-transform algorithm used by Pipe pathways, the same inputs which can be used to control the solution algorithm for Pipes also apply for Network pathways.

**Read more:** [Controlling the Pipe Solution Algorithm](#) (page 216).

## Summary of Limitations on the Use of Network Pathways

While Network pathways are versatile and powerful, they have the same limitations as Pipe pathways, which are worth summarizing here:

- Unlike Cell and Aquifer pathways, GoldSim does not apply solubility limits within Network pathways.
- If the properties of a fracture set (e.g., partition coefficients) change as a function of time, GoldSim has to use an approximation. The approximation is that species are discharged from a pathway based on the properties of the pathway *at the time the species (or their parents) entered it*.
- "Looping" reaction chains (A decays to B and B decays to A) are not permitted. Defining such reaction loops in a model that uses a Network pathway will result in a fatal error message.

## Saving Results for a Network Pathway

Network pathways produce the following outputs:

- the total mass of each species in the pathway;
- the average concentration of each species in the Reference Fluid exiting the pathway; and
- the mass flux of each species for all specified advective Outflows.

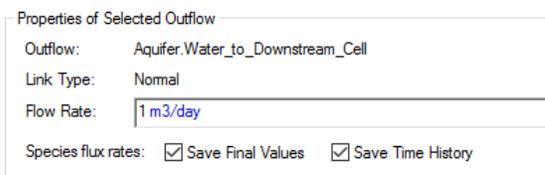
These outputs are all vectors by species. Reference Fluid concentrations have dimensions of mass/volume. Fluxes have dimensions of mass/time.

You specify that you wish to save these results in two different places:

1. Species masses in the pathway, concentrations in the Reference Fluid exiting the pathway, and discharges from Watch Groups are saved by clicking **Final Values** and/or **Time History** at the bottom of the Network pathway editing dialog:

Save Results		
Masses:	<input checked="" type="checkbox"/> Final Values	<input checked="" type="checkbox"/> Time History
Concentrations:	<input checked="" type="checkbox"/> Final Values	<input checked="" type="checkbox"/> Time History
Watch Group(s):	<input checked="" type="checkbox"/> Final Values	<input checked="" type="checkbox"/> Time History

2. Fluxes are saved by selecting a mass flux link in the Inflows or Outflows tab for a linked pathway and clicking **Save Final Values** and/or **Save Time History** at the bottom of the dialog:

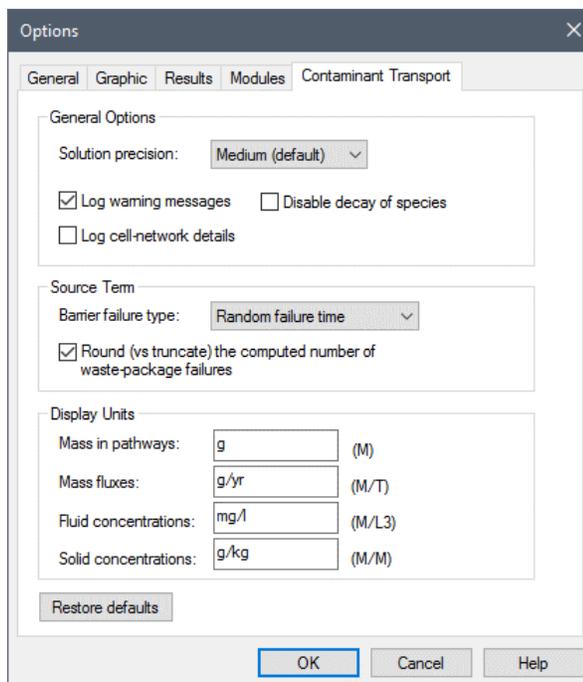


If you are running multiple realizations, the Time History box is ignored, and unless an output of the element is connected to a Time History Result element, no time history results will be saved at all for the element. In fact, in such a case, the Save Results section would look like this:

Final Values     Monte Carlo Histories

In this particular case, because the simulation involves multiple realizations, the “Time History” checkbox is replaced by a “Monte Carlo Histories” checkbox. This checkbox is grayed out, since it is only used for information purposes. You cannot edit it directly, and its appearance is completely determined by whether or not the output is connected to a Time History Result element. That is, in order to save time history results for a Network output when running multiple realizations, you must connect it to a Time History Result element.

The display units for masses, concentrations and fluxes for all pathways are specified in the **Contaminant Transport** tab of the Options dialog (accessed via **Model | Options...** from the main menu):



## Additional Comments on the Use of Transport Pathways

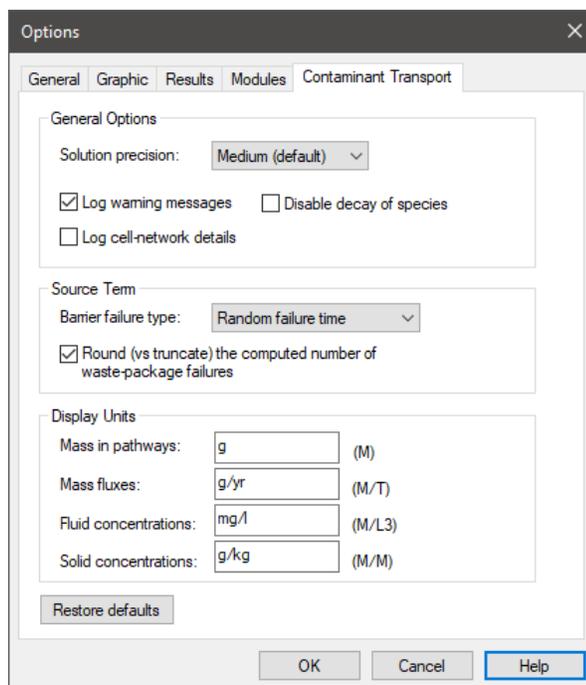
### Understanding the Solution Precision

The algorithms used by GoldSim to compute concentrations and fluxes associated with pathways are discussed in detail in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

Although it is not necessary for you to understand all of the details of these algorithms in order to use the Contaminant Transport Module, there is a **Solution precision** setting that you should be aware of in order to maximize the computational efficiency of your model and the accuracy of the results.

This setting can be found in the **Contaminant Transport** tab of the **Model | Options** dialog:



The **Solution precision** has three options: Low, Medium (the default) and High. The solution precision controls a number of different parameters used when solving the equations for pathways.

Most of these are associated with the solution of the matrix equations for Cells, and are described in detail in *Solving the Matrix Equations Numerically* in Appendix B. An additional parameter is associated with solving Pipe pathways, and is discussed in *Solution Technique for Pipe Pathways* in that Appendix.

Increasing the precision setting can make models run slower (and decreasing the precision setting can make models run faster). In most cases, you will not need to adjust this setting (and it is recommended that you leave it at the default of Medium).

There are two conditions, however, in which you may consider doing so:

- Under some conditions (typically associated with simulating solubility constraints and/or isotopes, it may be necessary to use High Precision.

**Read more:** [Understanding Solubility Calculations](#) (page 167).

- When using Pipe pathways to simulated very low dispersivity systems, it may be necessary to use High Precision.

**Read more:** [Controlling the Pipe Solution Algorithm](#) (page 216).

In addition, under some conditions (associated with rapidly changing media amounts in Cells, and Cells going empty), it may be appropriate to use Low Precision, although this may require shortening the timestep.

## Computing Pipe and Aquifer Pathway Concentrations Accounting for Transverse Dispersion

**Read more:** [Dealing with Changing Media Amounts in a Cell](#) (page 169).

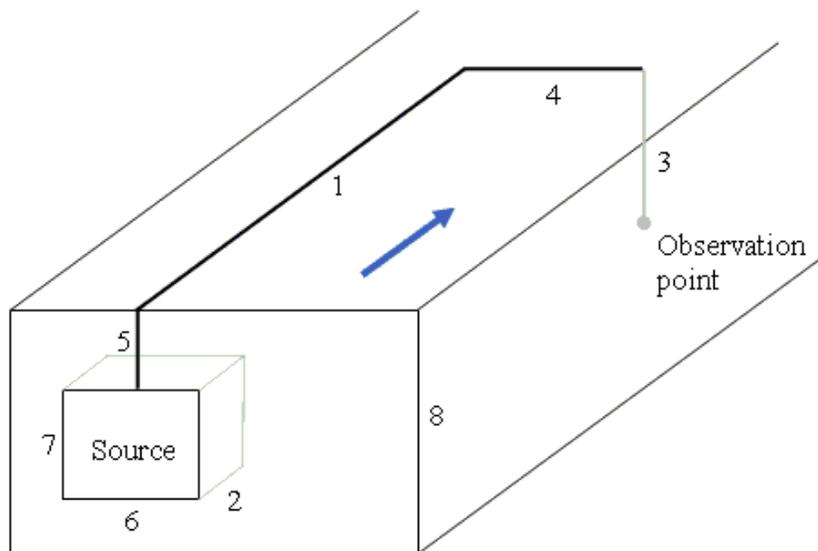
Since Aquifers and Pipes are meant to represent one-dimensional conduits, the concentration reported by these two pathways represents the average concentration discharging from the pathway, and any spatial variation in the concentration (perpendicular to the flow direction) is not represented.

In many cases, however, real world concentrations will vary spatially at the end of a flow path due to dispersion in the horizontal or vertical transverse direction and/or a source term which is not uniformly distributed across the area of the conduit being simulated.

In order to allow you to address this spatial variation, GoldSim provides a special function that returns a correction factor that can be used to multiply the Aquifer's or Pipe's concentration output in order to compute the actual (as opposed to spatially-averaged) concentration at an observation point at some distance perpendicular to the flow path at the end of the pathway.

The *Plume function* (which is analogous to other GoldSim functions like *sin* or *max*) has eleven input arguments which describe the properties of the pathway to which you wish to apply the correction, the size of the source, the dispersive properties of the pathway, and the exact location of the observation point. The source is assumed to be a point, rectangle or box centered on the midpoint of the flow path (the pathway), and the observation point is located at the end of the pathway some specified distance from the centerline.

The following diagram illustrates the various input arguments required by the Plume function.



The arguments are as follows (the numbers reference lengths in the figure above):

- Pathway Length (1)
- Pathway cross-sectional Area
- Source Length (2)
- Depth (vertical distance) from the ground surface (or top of the flowing zone) to the observation point (3)

- Horizontal (transverse) distance from the source center to the observation point (4)
- Depth of the top of the source (5)
- Width of the source (6)
- Vertical thickness of the source (7)
- Total thickness of the pathway being simulated (8)
- Horizontal dispersivity
- Vertical dispersivity

Note that the Plume function appears in the function list accessible by right-clicking in an input field and selecting Functions from the context menu (it can be found in the “Contaminant Transport” category). When you insert it, to assist in specifying the large number of inputs, GoldSim puts in temporary placeholders for the arguments (that you will of course need to replace with the actual input arguments):



When specifying these inputs, the following rules should be observed to ensure that the Plume function is physically consistent with the pathway concentrations to which you are applying it:

- The first three arguments should use the same values as those assigned to the pathway itself. Note that the pathway area does not impact the result (as long as the same pathway area is used in the Pathway and the Plume function).
- The product of the width and thickness of the source should not exceed the pathway Area.

The arguments to the Plume function can be links or expressions, and the output of the Plume function is dimensionless. The arguments can also be arrays (vectors or matrices), in which case the output of the function is an array. In such a case, not all of the arguments need to be arrays (arguments defined as scalars are applied to all items of the array). However, all arguments that are defined as arrays must have the same array labels sets.

Because you can specify the length, width and thickness of the source (and any of these can be zero), there is a great degree of flexibility in defining the dimensions of the source. A source can be defined as:

- A point;
- A horizontal area on the surface of an aquifer;
- A vertical area perpendicular to the pathway; or
- A volumetric box region.

The thickness of the aquifer (or river) is required because at a certain distance downgradient from the source, the vertical spread of the plume will encounter and reflect off the bottom. Further downgradient, it will reflect back off the top, and eventually the aquifer will be fully-mixed vertically. GoldSim automatically accounts for these reflections. Horizontal dispersion is assumed to be unlimited, however.

## Plume Function Solution Technique

The Plume function is based on an analytical approach for simulating the 3D transport of a contaminant plume. The solution integrates a point source over the specified horizontal and vertical source area (the Pipe and Aquifer have the solution for a source which is distributed longitudinally built in, so the Plume function only has to allow for transverse distribution and spreading). The point-source solution allows for transverse (horizontal and vertical) dispersion, and GoldSim automatically creates ‘mirror’ sources to represent the vertical reflections of the plume off the top and bottom of the aquifer.

The Plume function calculates transverse (horizontal and vertical) dispersion assuming that the observation point is at a (longitudinal) distance from the source equal to the total pathway length minus half of the source-length (i.e. at the center of the source-zone). If the source is distributed longitudinally over a distance that is a significant fraction of the total pathway length, this approximation will result in slightly underestimating the amount of transverse dispersion.

The details of the calculation are described in detail in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

## Comparison of Aquifers and Pipes for Simulating a One- Dimensional Pathway

Pipe and Aquifer elements both provide a way to simulate one-dimensional pathways (such as aquifers or rivers).

Although Aquifers and Pipes solve the same equation (using different methods), the boundary conditions that are applied at the end of the pathway differ, and this can cause differences in their results.

Aquifers can be assigned one of two boundary conditions:

- No dispersive/diffusive outflux allowed (only advection). This is the default option.
- Dispersive/diffusive outflux allowed, assuming a zero concentration in the receiving pathway. This would be appropriate, for example, if the downstream pathway represents a rapidly-flowing, “clean” pathway.

These two boundary condition options represent two possible extremes for the behavior of the system. The actual behavior of most real-world systems would be somewhere between these two extremes, although probably closer to either one or the other).

The boundary condition for the Pipe, on the other hand, is as follows:

Concentration goes to 0 as  $x$  goes to  $\infty$ .

Effectively, this allows dispersive/diffusive outfluxes, with a downstream concentration (immediately after the Pipe) that is not set to zero (as is the case for the Aquifer), but is actually quite close to the concentration in the Pipe (resulting in a low dispersive outflux).

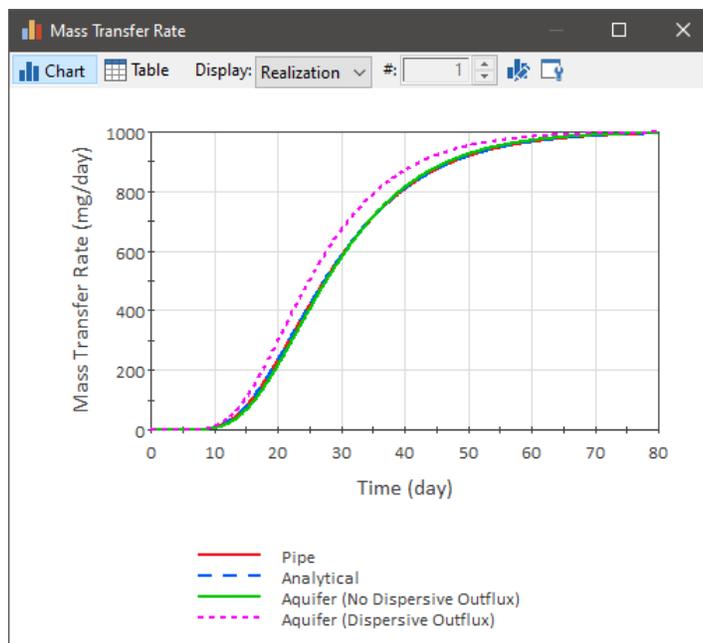
If you think carefully about this, you will realize that the Pipe boundary condition actually is close (but not identical) to the default Aquifer boundary condition (no dispersive flux).

To see this, let’s examine the breakthrough curves for one-dimensional pathways simulated using a Pipe and two different Aquifers (representing both boundary conditions).

The pathway is 50 m long, has a cross-sectional area of 1 m<sup>2</sup>, a dispersivity of 5 m, and a flow rate of 1 m<sup>3</sup>/day. The pathway is filled with a porous medium with a porosity of 0.3. At the upstream end, mass is added at a constant concentration of 1 mg/l. The Aquifer is based on 100 Cells, and the Pipe is

solved using High Precision. This particular example model, PathwayComparison.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

A comparison of breakthrough curves for these three cases is shown below:



**Note:** This plot also includes the analytical solution (Ogata and Banks, 1961), which has the same downstream boundary condition as the Pipe. The upstream boundary condition is close, but not completely identical to that for the Pipe or Aquifer, but at a sufficient distance any impacts are insignificant.

Akio Ogata and R.B Banks, 1961, “A Solution of the Differential Equation of Longitudinal Dispersion in Porous Media”, Geological Survey Professional Paper 411-A (<https://pubs.usgs.gov/pp/0411a/report.pdf>).

As can be seen, the analytical solution, the Pipe result and the Aquifer result assuming no dispersive outfluxes are essentially identical. The Aquifer result that allows dispersive outfluxes results in a faster breakthrough, however, since the zero concentration boundary condition that is assumed in the downstream pathway artificially increases the dispersive outflux (and would only be appropriate if the downstream pathway did in fact have a very low concentration due to rapid flushing).

Therefore, since the results in this simple case are similar, under what circumstances should one pathway be used instead of the other? Some general rules are provided below:

- If solubility limits are being approached within the pathway, you should use an Aquifer.
- If the pathways (or solute) properties, including flow rates, are changing significantly over the simulation, you should use an Aquifer.

- If you need to simulate processes that occur in fractured rock masses, such as matrix diffusion, you should use a Pipe.

Moreover, when using an Aquifer, the default boundary condition (no dispersive outfluxes) should be used unless the downstream pathway can in fact be assumed to be at a very low concentration relative to the concentration leaving the pathway (e.g., due to rapid flushing).

## Manipulating Pathway Outputs

It is worthwhile to mention three standard GoldSim elements that are likely to be useful for manipulating pathway outputs:

- **Sum element:** This element simply adds any specified inputs, producing a single output. Obviously, the inputs must be of the same type and dimension, and the output has the same type and dimension as the inputs. This element can be useful for adding pathway outputs (particularly fluxes or masses). For example, you may wish to compute the total amount of mass in a particular subsystem made up of several pathways, or the total flux rate entering a pathway from several other pathways.
- **Extrema element:** This element computes the highest or lowest value reached by its input as a function of time, outputting the "peak" or "valley". This can be useful, for example, if you wish to compute the peak concentration, or peak flux rate at a particular location in your system.
- **Integrator element:** In some cases, you may need to integrate the mass flux leaving a Pathway element using an Integrator. The mass flux leaving a Pathway element represents a rate over the *previous* timestep. However, Integrators treat their Rate of Change variable as if it is the rate over the *next* timestep. Hence, when using an Integrator to integrate the mass flux from a Pathway, to account for this difference, you must use the advanced properties the Integrator dialog to adjust how it integrates the Pathway's output. (See "Modifying How Integrators Treat the Rate of Change" in the **GoldSim User's Guide**).

## Mass Balance of Transport Media in Pathway Networks

The GoldSim Contaminant Transport Module is a mass transport model. That is, it tracks the masses of the species as it moves them through the system. It is important to understand, however, that *GoldSim does not impose a mass balance on the transport media*. Mass balances for transport media must be specifically imposed by the user.

For example, if two pathways discharge water into a third pathway, the volumetric flow rate out of the third pathway does not have to be equal to be the sum of the discharges from the two preceding pathways. The inherent assumption here is that if the flows do not sum to zero, it is because you know of an additional source (or sink) of flow that does not warrant explicit modeling.

If the flows of a particular medium out of the pathway are greater than the flows into the pathway, it implies that additional quantities of "clean" medium (containing no species concentrations) also enter the pathway. If the flows out of the pathway are less than the flows into the pathway, it implies that a quantity of the transport medium is leaving the system *without carrying any species with it*. This is generally not physically possible, although there are several special processes by which this could indeed occur (e.g., evaporation of water from a pathway; movement of a medium through a filter as it leaves the pathway).

Because this latter case is only physically reasonable under special circumstances, GoldSim will provide some limited warning messages. In particular, if the sum of the discharges for the Reference Fluid from a Cell,

Aquifer or Pipe is less than the sum of the recharges (advective mass flux links into the pathway) for the Reference Fluid, GoldSim will issue a (non-fatal) warning message. (Warning messages are not provided for External pathways or Network pathways.)



**Note:** Although this is a helpful warning, every model you build will have at least one Cell in which the Inflows exceed the Outflows. This is because all models have an “edge” or an “sink” where the model ends and you are no longer tracking mass. Hence, to avoid the warning message in this case, if the name of the Cell starts with the letters “sink” (case-insensitive), GoldSim will not issue the warning message for that Cell.



**Note:** For Cells, if the amount of the Reference Fluid has been defined in a manner that allows it to change (e.g., by defining the amount using a Pool or a Reservoir), GoldSim will not issue this warning message. This is because under these circumstances, it is assumed that you are properly tracking the volume of the fluid directly (and hence inflow/outflow imbalances are being explicitly accounted for). Moreover, the warning message is only written for the Reference Fluid. That is, if the Inflows to a Cell exceed the Outflows for any other medium in the Cell whose quantity is constant, the warning message is not written.



**Note:** GoldSim only provides a warning message if the absolute difference between the inflow and the outflow exceeds  $1\text{E-}10$  m<sup>3</sup>/sec AND the ratio of the absolute difference to the inflow exceeds  $1\text{E-}6$ .



**Note:** If you want to disable these warning messages completely, you can do so by clearing the **Log warning messages** checkbox in the **Contaminant Transport** tab of the **Options** dialog. Note, however, that this is not recommended.

It is strongly recommended that you specifically enforce media flow balances by specifying pathway flow rates and media volumes and masses in a manner that is physically consistent with the mechanics of the system being modeled.

**Read more:** [Coupling a Network of Cell Pathways to a Network of Reservoir or Pool Elements](#) (page 163).

## Moving, Copying and Cloning Pathways

Like other GoldSim elements, you can copy, move and clone Pathways. The following points should be noted regarding how Pathways within fluxes are treated when they are moved, copied or cloned:

- When you copy a pathway, any outfluxes it has will be copied with it. Hence, if a flux exists from Cell1 to Cell2, and Cell1 is copied, the new Cell will also have a flux link to Cell2.
- When you copy a pathway, any influxes it has will *not* be copied with it. Hence, if a flux exists from Cell1 to Cell2, and Cell2 is copied, the new Cell will *not* have a flux link from Cell1.
- When you move a pathway it always retains all influxes and outfluxes.

- When you clone a pathway, all outfluxes are cloned with it; none of its influxes, however, are cloned.
- When you create a clone of a pathway, its outfluxes will link to the same pathway to which the original pathway was linked. If you wish to clone an entire system of pathways, you should place the system in a Container and clone the Container.

### Copying Pathways Between Models

In many cases, you may wish to create different portions of your model in different model files. For example, one individual may be working on one part of your model (a particular subsystem), while another is working on a different subsystem. At some point, you would then want to combine the various subsystems into a single model file.

GoldSim allows you do so by simply opening two instances of GoldSim (each with a different file), copying the desired element (including entire Containers) to the clipboard, and then pasting it into the other model.

Copying elements between models in this way is discussed in detail in Chapter 3 of the **GoldSim User's Guide**.

When you are copying and pasting pathways in this manner, however, there is an important limitation that GoldSim imposes that you must be aware of: You should only copy pathways between models if the two models have identical species.



**Warning:** GoldSim will actually allow a pathway copy/paste operation if the species lists in the models have the same *number* of items. GoldSim does not automatically check to see if the items are identical. It is strongly recommended, however, that you ensure that the species lists are identical before copying and pasting pathways between models.

### Placing Pathways in Conditional or Looping Containers

As discussed in Chapter 10 of the **GoldSim User's Guide**, you can create conditional Containers in GoldSim. This allows you to make the Container and all of its contents inactive when specific conditions are met. Elements in an inactive Container are “dormant”. There are some special rules that govern the use of CT/RT elements in conditional Containers:

- Even if a Species or Media (Fluid or Solid) element is in an inactive Container, these elements are never deactivated. If one of these elements is inside an inactive Container, the element will ignore this fact.
- Species elements, Pathway and Source elements can exist within a conditional Container, but you cannot deactivate the Container. That is, these elements can start in Containers that are initially inactive, but cannot exist in Containers that start active, and subsequently deactivate. Trying to deactivate a Container with a Pathway, Source or a Species element will result in a Fatal Error.
- If an active Pathway is linked (via an outflow) to a Pathway that is initially inactive, a Fatal Error will be displayed
- If a Pathway or Source is initially inactive, no decay calculations are carried out within the Pathway or Source until it is activated.

In addition, although GoldSim does not specifically prevent it, Cells in the same cell net should never be spread between active and inactive Containers, as this is likely to lead to unrealistic behavior and results.

## Simulating Looping Pathway Networks

As discussed in Chapter 10 of the **GoldSim User's Guide**, you can create looping Containers in GoldSim that carry out iterative calculations. As a general rule, you should not place any CT/RT elements in a looping Container.

As part of the solution algorithm for pathways, GoldSim analyses and sorts cell nets, Aquifer pathways, Pipe pathways, External Pathways, and Network pathways in terms of the "upstream-downstream" direction of media flows. (In this respect, one can think of a cell net as another type of pathway).

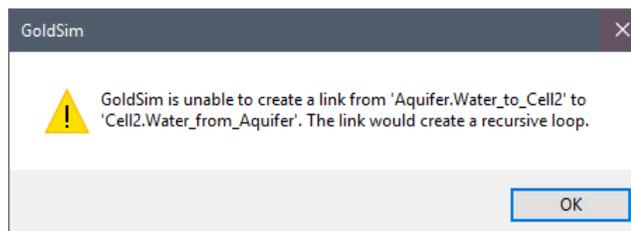
**Read more:** [Understanding Cell Nets](#) (page 165).

Typically, you need not be concerned about this sequencing of pathways and nets. However, in some situations, you will be prompted to take action to rectify a sequencing problem. In particular, if the upstream/downstream sequencing of pathways and nets is ambiguous or can't be explicitly determined (e.g., the network "loops"), GoldSim will issue a warning message saying that "there is a recursive loop".

The screen below shows an example of a network which cannot be unambiguously sequenced:

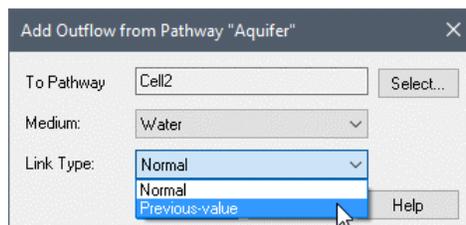


GoldSim would issue a warning when you tried to connect Aquifer to Cell2:



In order to create the mass flux link, it (or another link in the loop) must be created as a **previous value mass flux link**. A previous value mass flux link specifies that the previous timestep's value be used instead of the current timestep's value. This corrects the sequencing problem. Note, however, that as a result, a one timestep delay in the propagation of mass is created at the point that the previous value link is inserted in a pathway network.

When you create a mass flux link, you can select the link type in the dialog that is displayed when you select the pathway to link to:



**Read more:** [Creating and Editing Advective Mass Flux Links](#) (page 91).

Note that if you subsequently display the Influence dialog containing the link (by double-clicking on the influence), GoldSim will indicate that the link is a Previous Value link:





---

# Chapter 5: Contaminant Sources

**Source:** A point, line or area at which mass or energy is added to a system, either instantaneously or continuously.

*McGraw-Hill Dictionary of Scientific and Technical Terms*

## Chapter Overview

This chapter describes the use of Sources in GoldSim. Within GoldSim, there are three ways to introduce mass into the system:

- An initial mass or a rate of addition of mass can be directly specified for one or more pathways in the system;
- A discrete addition can be made to one or more Cell pathways; and/or
- The user can define the properties of one or more *sources*, and based on the properties, GoldSim will compute rates of release of mass from the source(s) to specified pathways.

You will often need to only use the first two methods to introduce mass into your model. In many cases, however, it may be necessary to explicitly model a source such that the effect of the barriers (such as drums or boxes) and/or a waste matrix (e.g., cement) in which the species are contained can be represented more accurately.

This is particularly important when simulating the behavior of proposed or existing waste disposal facilities which have, as part of their design, engineered packages or containers in which the waste is placed prior to disposal.

The Source element provides this capability.



**Note:** The Source element is only available in the RT Module.

---

## In this Chapter

This chapter discusses the following:

- Using Contaminant Sources
- Defining a Source: Overview
- Defining the Level of Containment
- Defining Source Inventories
- Associating Cells with a Source
- Defining Barrier Failure
- Source Outputs

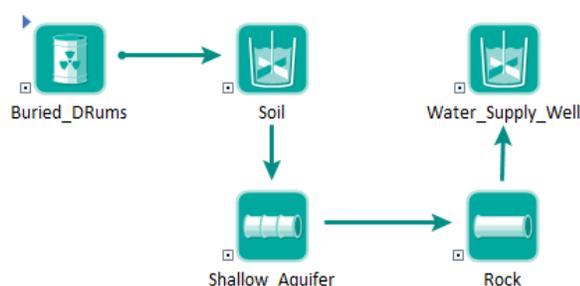
- Instantaneously Moving Mass from a Source
- Source Example Models
- Viewing a Source in the Browser
- Saving Results for a Source

## Using Contaminant Sources

### What is a Source?

Within GoldSim, the definition of what is meant by a “source” is completely determined by the user. A “source” may represent an entire landfill, or a single buried drum; a group of leaking underground tanks or a complex engineered facility. In a given system, multiple sources may exist.

The key point is that a Source element inputs contaminant mass to the pathway network (which subsequently transports mass through the system), as shown below:



*This Source element “Buried\_Drums” provides mass input to the Cell pathway called “Soil”.*

In effect, a Source can be viewed as a “black box” whose outputs are release rates for each species in the system to one or more transport pathways.

A Source allows you to define the properties and characteristics of the various contaminant sources in your system, and based on these, computes the resulting release rates to specified transport pathways. The properties and characteristics that you must specify for each Source are as follows:

- **Containment:** Is part or all of the species mass at the Source initially present within barriers of some sort (e.g., drums, boxes) which must fail before any of the contaminants can be released? If so, what is the rate at which the containers fail?
- **Inventory:** What is the initial quantity of each species at the source? Where is it located within the Source (relative to any barriers that may exist)?
- **Waste matrix:** Is part or all of the contaminant mass at the Source bound within one or more matrix materials of some sort (e.g., grout, metal) which must degrade to some extent before any of the contaminants can be released? If so, what are the degradation rates of these materials?
- **Mass Transfer:** What are the physical and chemical characteristics of the Source which control the rate at which contaminant mass (once it is liberated from any containers or matrix materials) can be transported through and away from the source?
- **Connections to the Pathway Network:** When mass leaves the Source, to which pathways does it discharge?

## When Should You Use a Source Element?

Once the nature of each Source is specified in this manner, the resulting mechanisms controlling release can be simulated.

The rule for whether or not you need to use a Source element in your model is relatively straightforward: *If you cannot represent the introduction of mass into your model (i.e., the source term) in an accurate manner using a simple equation, you should probably use a Source element.*

That is, if you can't describe the introduction of mass into your system by using an initial or boundary condition (or a discrete change) in a pathway, you should use a Source element. This will often be the case if 1) your source involves barriers which fail over time; 2) your source includes one or more matrix materials which release species mass as they degrade; and/or 3) the source term is modified by reactions (e.g., decay and ingrowth). If any of these processes are active, describing the source term using simple algebraic equations becomes difficult, if not impossible (since in these situations, representing the source term accurately involves the solution of integrals and/or coupled systems of equations). These processes, however, can be explicitly represented using a Source element.

## Processes Modeled by a Source

GoldSim explicitly represents two processes which control release of mass from a Source:

1. *exposure* of the contaminant mass within a Source; and
2. *transport* of exposed contaminant mass through and away from the Source.

The processes are discussed below.

## Exposure of Contaminant Mass within a Source

The term *exposure*, as applied to a Source, has a specific meaning within GoldSim. In particular, species mass in a Source is considered to be *exposed* if it is available for mass transfer within and away from the Source. If a contaminant is present within an intact barrier, or bound within intact matrix material of some sort (e.g., grout, metal, glass), it is not available for mass transport, and hence is considered to be *unexposed*. The mass cannot be transported until it is physically liberated from barriers and/or matrix material present at the Source. Hence, within a Source, exposure is controlled by two processes:

- **Loss of Containment.** The mass can be specified to be present in the Source in discrete *packages* (e.g., 100 separate drums). For each individual package, two layers of containment (barriers) can be explicitly considered to exist (e.g., a drum and a liner within the drum). The mass can be distributed in various places within the barrier system inside a package (e.g., between the outer and inner barriers, inside both barriers). Barrier failure rates are described in terms of density functions of failure frequency (e.g., the rate of drum failures).
- **Degradation of waste matrix.** All or portions of the species mass within the Source can be specified to exist within one or more matrix materials, such as cement, grout, solidified glass, or metal. Species which are bound in such a matrix are not released until the matrix itself degrades (e.g., dissolves, corrodes or alters) in some manner. Release of species mass from the matrix is then assumed to be congruent with the degradation of the matrix.

These two processes together determine the *rate of exposure* of contaminant mass within a source.

***Transport of Exposed Mass Through and Away from the Source***

Once mass is exposed within a Source, it is available for transport within and away from the source. GoldSim allows both advective and diffusive transport mechanisms to be explicitly represented. Mass transport within and away from a source is controlled by the following:

- **Partitioning.** The Source can contain multiple fluid and solid transport and storage media (e.g., water, oil, rust, soil), with partition coefficients between the various media. Exposed contaminant mass will be partitioned between the various media within the Source based on the partition coefficients and the masses or volumes of the media. This in turn, will affect transport rates.
- **Solubility constraints.** Solubility limits for the contaminants can be specified within the Source. Precipitated mass can only be transported via advection of the solid media it has precipitated onto.
- **Mass transfer.** Media flow rates through the Source, geometric considerations, and contaminant properties (e.g., diffusivities) control the advective and diffusive mechanisms by which exposed mass can be transported.

The transport of mass through and away from a Source is actually implemented within GoldSim by associating (i.e., linking) one or more Cell pathways with each Source. Cells that are associated with Sources in this way take on some special properties.

***Comments on Competition Between Exposure and Mass Transport Rates***

Mass exposure and mass transport can be viewed as competing processes with regard to controlling the rate of release of a species from a Source. Typically, one of these processes dominates for a given species in a Source.

For example, for a Source consisting of a highly insoluble species spilled directly onto the ground surface, the concept of containment or matrix degradation is not applicable, since the contaminant is exposed immediately and available for mass transport. In this case, the release rate would be equal to the mass transport rate, which in turn is controlled by the solubility limit.

If, however, water containing a soluble species (e.g., chloride) was stored in a number of drums which gradually failed over time, then the exposure rate (i.e., the rate of drum failure) would likely control release since the species would be transported away as quickly as it was exposed.

In the first case, you would know beforehand that mass transport always controls release, and you could therefore simulate the system without even using a Source. Note, however, that within a Source, different species could be controlled by completely different mechanisms, and you may not be able to specify which mechanism is dominant for a given species beforehand. Moreover, the dominant mechanism may change for any given species from realization to realization.

For example, if the contaminated water within the drums contained a relatively insoluble species (e.g., lead) in addition to the chloride, then, depending on the solubility and the container failure rate, the release rate for this species could be controlled by mass transport considerations, even though the species was being exposed relatively gradually due to drum failure. This is because the low solubility could limit the rate at which mass was transported away. In such a case, exposed lead would simply “accumulate” at the Source as more drums failed, with the release rate from the Source remaining relatively steady due to the solubility limitation on mass transport.

## Defining a Source: Overview

The four steps required to define a Source are as follows:

1. Specify the *Level of Containment* of the Source. This consists of defining the **Number of Packages** into which the mass in the Source is to be discretized, and the **Number of Barriers** defined for each package.. The Number of Packages represents the number of discrete containers represented by the Source. Inventories (the amount of contaminant mass in the Source) are defined per package. The primary purpose of discretizing the Source into packages is to facilitate simulation of barrier failure (containment). Packages can be defined to have no barriers (e.g., soil disposed of directly in a trench), a single barrier (e.g., waste disposed of in drums); or a double barrier (e.g., an engineered waste package containing one or more secondary containers inside).
2. Define the *inventories* in each package in the Source. An inventory consists of a vector of species masses in a specific location relative to the barriers (e.g., inside the outer barrier, inside the inner barrier). Inventories can be optionally specified as being bound within a waste matrix (in which case a *matrix degradation* rate must be specified). Multiple inventories can be defined for a Source.
3. Define the *Associated Cells* for the Source. Associated Cells are specialized Cell pathways which are associated with the Source and are used to simulate the transport of mass through and away from a Source.
4. If you have specified that your Source has barriers, define the barrier *failure distributions*. Failure distributions must be defined for each barrier you have specified.

The editing dialog for a Source is shown below:

Source Properties: Drums

Definition Graphics Information

Element ID:  Appearance...

Description:

Properties

Number of Packages:

Number of Barriers:  Outer Barrier... Inner Barrier...

# Packages failed by events:

Source Inventory Settings:  Number of Inventories: 1

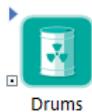
Inventory Cells

Cell	Balance	Fraction of Balance	
Cell1	1	1	

Save Results

	Final Values	Time History
Unexposed Mass in Source:	<input type="checkbox"/>	<input type="checkbox"/>
Cumulative Releases to Inventory Cells:	<input type="checkbox"/>	<input type="checkbox"/>
Number of Failed Packages:	<input type="checkbox"/>	<input type="checkbox"/>

Note that a Source element is actually a specialized type of Container. This can be recognized by the triangle in the upper left-hand corner of the element:



Sources have **Graphics** and **Information** tabs associated with all Containers. Source Containers can also be localized

---



**Note:** Containers are discussed in Chapter 3 and localized Containers are discussed in Chapter 10 of the **GoldSim User's Guide**.

---

The Associated Cells for the Source element are defined by inserting them inside the Source Container.

The detailed steps required to define a Source are discussed in detail in the following sections.

## Defining the Level of Containment

The first two fields in the Source dialog (**Number of Packages** and **Number of Barriers**) determine the level of containment for the Source:

**Number of Packages:** This is the number of packages in the Source. As such, it represents the degree to which the mass in the Source is discretized (the default value is 1 package). Each package in a Source is identical with regard to its inventories and failure distributions.

The number of packages should be specified as an integer. Non-integer values are automatically truncated (internally) by GoldSim.

The purpose of discretizing the Source into packages (and subsequently defining barriers) is to facilitate simulation of barrier failure (containment). If you are not simulating barriers, simply specify the Number of Packages as 1.

---



**Warning:** If you are modeling barriers, the number of packages should be carefully specified. Many Source properties are defined on a *per package* basis (e.g., inventory per package). In addition, the number of packages can have important implications on the behavior of the Source.

---

**Read more:** [Controlling the Outer Barrier Failure Algorithm](#) (page 280).

**Number of Barriers:** Packages can be defined to have no barriers (e.g., soil disposed of directly in a trench), a single barrier (e.g., waste disposed of in drums); or a double barrier (e.g., an engineered waste package containing one or more secondary containers inside).

This list box therefore has three options: none, single, or double.

If "none" is selected, it indicates that there are no barriers in the package (and the **Outer Barrier...** and **Inner Barrier...** buttons will be disabled and grayed out).

If "single" is selected, it indicates that there is a single layer of containment (a single outer barrier) for the package. In this case, the **Outer Barrier...**

button will be enabled, and the **Inner Barrier...** button will be disabled and grayed out.

If "double" is selected, it indicates that there are two layers of containment for the package (one or more inner containers within an outer container). In this case, both the **Outer Barrier...** and **Inner Barrier...** buttons will be enabled..

## Defining Source Inventories

The species masses that are present in a Source are defined by specifying *inventories*. Multiple inventories can be defined for a Source. Each inventory has a specific location within the Source (relative to the barriers), although multiple inventories can coincide in the same location. Also, Inventories can optionally be specified as being bound within a waste matrix (in which case a *matrix degradation* rate must be specified).

The amount of mass in each inventory, coupled with its location and its matrix degradation rate, determines the rate at which its mass is exposed. The mathematical details of how the exposure rate for an inventory is calculated (as a function of barrier failure rates and matrix degradation) are described in Appendix E.



**Note:** An inventory specifies the amount of species mass at a specific location in a *single* waste package.

**Read more:** [Appendix E: Details of Source Computations](#) (page 399).

### Specifying an Inventory

Inventories are defined by pressing the Source Inventory Settings **Edit...** button in the Source dialog. The following dialog will be displayed:

Inventories can be added and deleted using the **Add Inventory** and **Delete Inventory** buttons. (Note, however, that you must have at least one inventory). You can move between existing Inventories using the **Previous** and **Next** buttons.

You can assign a **Description** to each inventory. This is not used by GoldSim and is for documentation purposes only. For each Inventory, the following must be specified:

**Species Mass:** This is the initial amount of species mass associated with this inventory. It represents the amount of mass in a single package. It must be a vector by species with dimensions of mass. The values must be non-

negative and should not vary with time. If an Inventory does vary with time, only the initial values will be used.



**Note:** If you are simulating radioactive species (using the RT Module) and your input inventories are in terms of activity (Ci or Bq), you can easily convert these to mass by dividing the inventory vector by the specific activity vector:

---

$$\text{Inventory} / \text{Species.Specific\_Activity}$$

---

**Location:** This is a list-box with two options: "Outer" and "Inner". It specifies the location of the Inventory relative to the barriers. "Outer" means within the outer barrier, and "Inner" means within the inner barrier. Note that if you have no barriers, this input is grayed out. Similarly, if you have only a single barrier, only the "Outer" option is available.

**Waste Matrix:** This is drop-list that determines whether or not the Inventory is bound in a matrix, and if it is, the manner in which the matrix is assumed to degrade. There are four options in the drop-list:

**None:** The Inventory is not bound within a matrix (the default).

**Specified lifetime:** The inventory is bound in a matrix, and the matrix degrades with a specified lifetime. The lifetime is specified in the field directly below the drop-list. The lifetime represents the time period over which the matrix is degraded at a uniform rate. The value must be non-negative and have dimensions of time.

**Specified degradation rate:** The inventory is bound in a matrix, and the matrix degrades with a specified rate. The rate is specified in the field directly below the drop-list. The rate must be a fractional degradation rate. That is, it represents the fraction of the existing mass which degrades per unit time. The value must be non-negative and have dimensions of inverse time.

**Congruent dissolution:** The inventory is bound in a matrix, and the matrix degrades based on solubility-limited dissolution. GoldSim identifies the largest single species in the inventory, and treats this as the matrix material. Upon barrier failure, the matrix is then degraded at a rate that keeps the matrix species at its solubility limit within all Inventory Cells.

Note that when matrix degradation is specified (i.e., the latter three cases), the following two points always apply:

- Species mass is exposed congruently with the degradation of the matrix.
- Matrix degradation in a package does not start until the barriers for the package have failed.

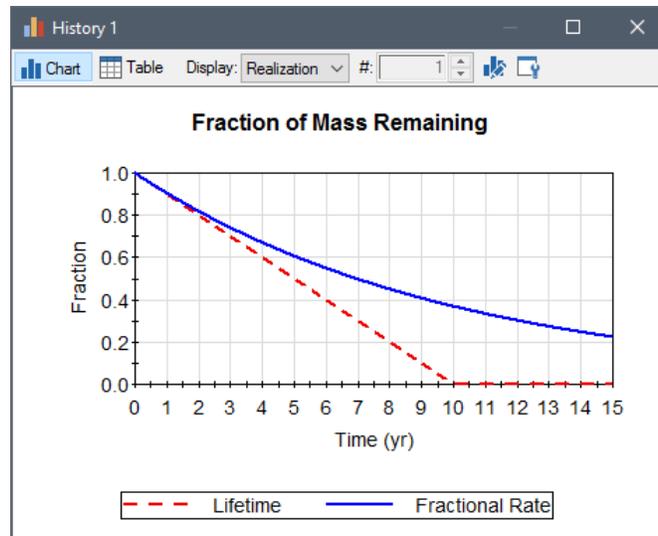
**Read more:** [Understanding Matrix Lifetimes and Fractional Degradation Rates](#) (page 266); [Understanding Congruent Dissolution of the Waste Matrix](#) (page 268).

### ***Understanding Matrix Lifetimes and Fractional Degradation Rates***

The first two options for defining matrix degradation rates in the Source Inventories dialog are:

- Specify a fractional *degradation rate* (with units of inverse time). This represents the fraction of the existing matrix mass which degrades per unit time.
- Specify a *matrix lifetime* (with units of time). This represents the time period over which the matrix is uniformly degraded.

It is important to understand that a fractional degradation rate and a matrix lifetime behave quite differently in terms of the amount of contaminant mass remaining (i.e., the amount of unexposed mass). If you use a (constant) fractional degradation rate, the amount of mass remaining to be exposed decreases exponentially, while if you use a lifetime, the mass decreases linearly:



In this example, one Source is represented using a Matrix Lifetime of 10 years, while the other Source is represented using a (fractional) Matrix Degradation Rate of 1/10 yr (i.e., 10% per year). As can be seen, because the fractional degradation is exponential, it actually takes longer than 10 years to expose all of the mass.

In reality, matrix degradation rates are typically a function of available surface area, and as such, are often quantified (e.g., in experiments) in units of mass/area/time (referred to as an *absolute degradation rate* in the following discussion). A fractional degradation rate could then be computed as the product of the absolute degradation rate and the *specific area* of the matrix (defined here as the area per unit mass).

Note that if you assume that the absolute degradation rate is constant in time, the fractional degradation rate will only be constant in time if the specific area stays constant. This is valid if degradation rates are very small, but for higher rates, this is likely to be a poor assumption. This is because for nearly all possible geometric configurations, the specific surface area of a mass will typically increase with time as the material degrades (although it could potentially stay constant or even decrease if the shape of the mass changes significantly as it degrades).

Countering this to some extent is the fact that it would not be unusual for the absolute degradation rate to decrease over time (e.g., due to the build up of corrosion products, etc.).

Typically, due to the considerable uncertainty in the actual geometry of the matrix, as well as uncertainty in long-term absolute degradation rates, it is

difficult to explicitly model the time variability of the degradation rate, and specification of a constant (but uncertain) fractional degradation rate or, alternatively, an uncertain lifetime is appropriate.



**Note:** If you do choose to model time dependency of the degradation rate, note that degradation is not likely to be a function of time; rather it is likely to be a function of the *time since the package failed*. Although GoldSim does not start degradation until a package fails, there is no way to reference the individual package failure times when defining the degradation rate. Hence, you should only specify the degradation rate as a function of time if it actually is a function of time (rather than time since failure). This would be appropriate, for example, if all packages failed at the same time *and* you explicitly accounted for the failure time in the equation for the degradation rate.

---

### **Understanding Congruent Dissolution of the Waste Matrix**

The third (and most advanced) option for defining matrix degradation rates in the Source Inventories dialog is to assume that the matrix degrades based on solubility-limited dissolution.

To simulate this, GoldSim identifies the largest single species in the inventory, and treats this as the matrix material. Upon barrier failure, the matrix is then degraded at a rate that keeps the matrix species at its solubility limit within all Inventory Cells (at least until the matrix is completely dissolved).

This method more accurately represents that actual degradation process for many types of systems in which the degradation rate is a function of 1) the matrix material's solubility; and 2) the rate of transport of dissolved matrix material away from the waste package. For systems that have low flow rates, this process of solubility and transport-limited matrix degradation can represent a significant barrier to release of contaminant species. It would also be difficult, if not impossible, to capture this process accurately using one of the other two matrix degradation methods.

There are requirements that must be met in order to use this option:

- The Inventory Cells must contain Water or some other Fluid. If no Fluid is present, the matrix will not degrade.
- The matrix species must have a non-zero solubility. If the solubility of the matrix species is zero, the matrix will not degrade.
- One species in the inventory should be larger than all of the others combined (in terms of mass), and this species is automatically defined as the matrix material. If this is not the case, GoldSim will select the species with the largest mass, and add a warning message to the Run Log.
- If Inventory Cells inside different Sources are part of the same Cell net, for any Sources that have congruently-dissolved matrices, the same species must represent the waste matrix.

An overview of the solution algorithm is discussed in Appendix E.

**Read more:** [Appendix E: Details of Source Computations](#) (page 399).

## **Associating Cells with a Source**

Once mass is exposed, it can be transported through and away from the Source. GoldSim uses the Cell pathways to represent this process. In particular, one or

more Cell pathways must be specified as being *associated* with the Source. Cells are associated with a Source by placing them inside a Source Container.

**Read more:** [Using Cell Pathways](#) (page 119).

One or more of the Associated Cells are further specified as being *Inventory Cells*. Exposed mass from the Source is distributed to the Inventory Cells. You decide which Cells are to be associated with a particular Source, and how the exposed mass in a Source is split among its Inventory Cells.

The Associated Cells for a Source are intended to physically represent a *single package* within the source. They behave in a special way in order to represent mass transport from a Source consisting of multiple packages. In particular, GoldSim automatically scales some properties of these Cells to represent the presence of multiple packages. Associated cells are connected (advectively and diffusively) to other (unassociated) Cells in the system in order to link the Sources into the pathway network.



**Warning:** You should not place other kinds of pathways inside a Source. Only Cell pathways should be used inside a Source element.

---

## Defining Associated Cells

Source elements are actually a specialized typed of Container. Like all other Containers, they can contain other elements.



**Note:** Containers are discussed in Chapter 3 of the **GoldSim User's Guide**.

---

This property of Sources is used to define associated cells. In particular, any Cell pathway inside a Source is considered to be associated with the Source.

Because Associated Cells have some special properties, you need to carefully decide which Cells are placed inside the Source Container (and hence associated with the Source), and which are placed outside the Container.

**Read more:** [Understanding the Behavior of Associated Cells](#) (page 271).

By definition, all Sources must have at least one associated Cell. Therefore, by default, when you create a new Source, GoldSim automatically creates it with a new Cell inside. This Cell is also automatically defined as an Inventory Cell.

**Read more:** [Defining Inventory Cells](#) (page 270).

In addition to Associated Cells, you can place any other elements that are logically associated with the Source (e.g., any of the input parameters for the Source) inside the Source element.



**Note:** It is strongly recommended that you do not add other kinds of pathways to a Source. A Source should only contain Cell pathways.



**Note:** A Source cannot contain another Source. If you try to do this, GoldSim will prevent it and display a warning message.

---

## Defining Inventory Cells

At least one of the Associated Cells for the Source must be defined as an *Inventory Cell*. Inventory Cells are the Cells into which exposed mass from the Source will be released. Note that not all Associated Cells need to receive mass directly from the Source (i.e., they do not all have to be Inventory Cells).

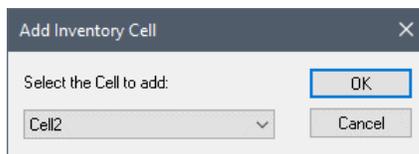
Inventory Cells are specified in the Source dialog:

Cell	Balance	Fraction of Balance
Cell1	1	0.5
Cell2	0.5	0.4
Cell3	0.3	1

By definition, all Sources must have at least one Inventory Cell. Therefore, by default, when you create a new Source, GoldSim automatically creates it with a new Associated Cell inside, and this Cell is automatically defined as an Inventory Cell. The Cell is assigned a default name (e.g., Cell1), which of course, you can subsequently change.

Additional Inventory Cells are added in one of two ways.

1. If you press the top button adjacent to the Inventory list (the green plus sign), the following dialog for inserting a new Inventory Cell will be displayed:



The list-box includes all of the Cells in the Container that have not already been defined as Inventory Cells. After selecting a Cell and pressing **OK**, the Cell will be added to the list of Inventory Cells.

2. If you press the middle button adjacent to the Inventory list (circled plus sign), GoldSim will immediately create a new Cell inside the Source, insert it into the list of Inventory Cells, and display the property dialog for the Cell.

You can remove a Cell from the list of Inventory Cells by pressing the Remove button adjacent to the Inventory list (the red X). Note that removing a Cell from the Inventory list does not delete the Cell from the model.

This Inventory list itself has three columns. The first contains the names of the Cells (and cannot be directly edited).

The second column (which is also not editable) shows the "balance", or the maximum fraction of exposed mass which could be assigned to that particular Inventory Cell.

The third column represents the fraction of the balance of the exposed mass that you wish the Cell to receive. Note that because it represents the fraction of the balance, this is a *relative fraction*, rather than an actual fraction. For example, in the screen shown above, Cell1 would receive 50% of the exposed mass, Cell2 would receive 40% of 0.5 = 20% of the exposed mass, and Cell3 would receive 100% of .3 = 30%.

Note the "fraction of balance" for the last Cell in the list cannot be edited (i.e., is always 1).

## Understanding the Behavior of Associated Cells

Although this approach is complex, specifying the fractions in this way ensures that the actual fractions always sum to 1 (even if some of the fractions are specified probabilistically).

An associated Cell is intended to represent the behavior of a *single* package within a Source. If a Source has multiple packages, GoldSim automatically scales some of the properties of the Associated Cells in order to represent that the Cells contain the exposed mass of multiple packages.

The Associated Cell properties that are scaled internally by GoldSim are as follows:

- the *volume* and *masses* of the media in the Cell;
- the *flow rate* for advective mass flux links from the Cell; and
- the *diffusive area* for diffusive mass flux links to/from the Cell.

These properties are dynamically multiplied by the number of failed packages. Hence, at any given time in a simulation, an Associated Cell actually represents the group of all the packages which have failed up to that time. In effect, GoldSim accounts for the presence of multiple packages by simply increasing the size of the Associated Cells.

An implicit assumption of this approach is that at any given time, all of the exposed mass within a Source is evenly distributed among the failed packages. In reality, the exposed mass may be concentrated in a fraction of the failed packages (e.g., those that have failed recently). In cases where solubility limits are involved, assuming that the exposed mass is evenly distributed throughout all the failed packages can be conservative with respect to release rates (i.e., result in an overestimate for the rate of mass transfer). This is because if mass transfer from a single package is actually limited by solubility considerations, spreading the same mass over a number of packages could have the effect of artificially negating this limitation.

In order to avoid this assumption and more accurately simulate the mass transfer within a source, it would be necessary to represent every package using a separate set of Associated Cells. If only a limited number of packages exist (e.g., 10), this could be accomplished by defining a separate Source for each package. If the number of packages numbers in the hundreds or thousands, however, such an approach would quickly become computationally impractical.



**Note:** Because properties of Associated Cells are scaled internally with the number of failed packages, you should take great care when creating mass transfer connections in which mass could move *into* an Associated Cell. In most cases, such a connection would not make sense physically (since the incoming mass transfer rate would only be affected only by *failed* packages inside the Source). As a result, typically, it would only be physically meaningful to create mass transfer connections *into* Sources in which all packages are assumed to fail immediately.

---

## Defining Barrier Failure

Source mass can be specified to be present in discrete packages (e.g., 100 separate drums). For each individual package, two layers of containment (barriers) can be explicitly considered to exist (e.g., a drum and a liner within the drum).

## Understanding Barrier Failure

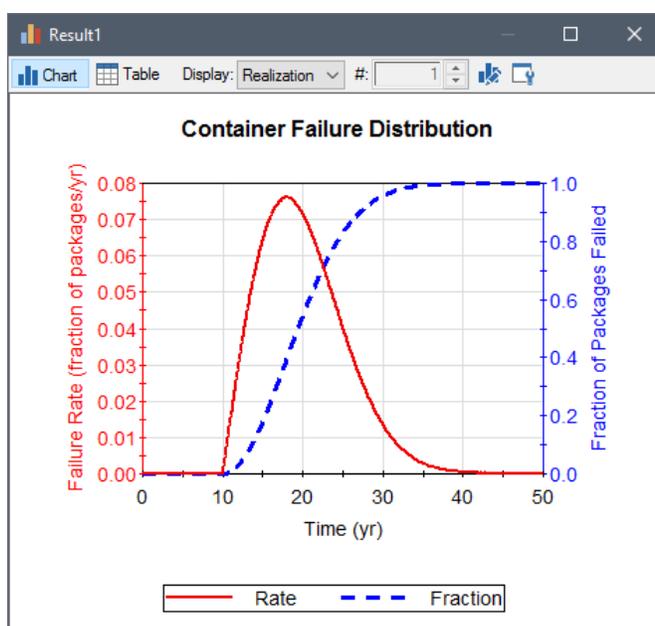
**Read more:** [Defining the Level of Containment](#) (page 264).

Mass is not released from the Source until the barriers have failed. Barrier failure rates are described in terms of density functions of failure frequency (e.g., the rate of drum failure).

The sections below describe the details of how you can define barrier failure.

If a number of steel drums (or some other type of container) were buried in the ground (or left sitting at the ground surface), at some point in time they would begin to fail (i.e., leak). It is highly unlikely, however, that the containers would all begin to leak at the same time. Rather, there would be temporal variability in their failure times (i.e., some containers would fail early, and some would fail at later times). If there were a large number of containers considered, the distribution of failure times would likely be relatively continuous. This variability in failure times could be quantified by defining a *failure distribution*.

Such a failure distribution is shown below:



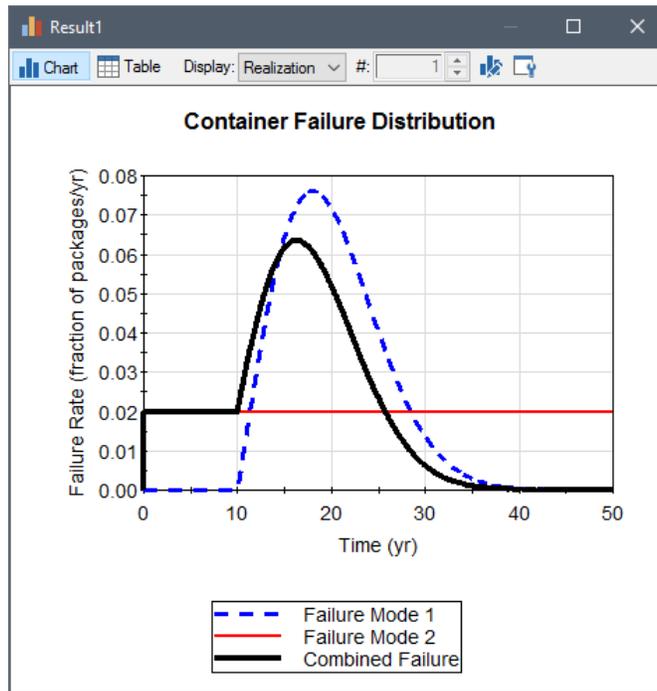
A failure distribution is a density function of failure frequency. The figure above shows two views of a failure distribution. The solid line (left axis) shows the fraction of containers failing *at a given time*. This can be thought of equivalently as a failure rate plotted versus time. The dashed line (right axis) represents the integral over time of this curve, which is the actual fraction of containers that had failed by a given time.

You represent barrier failure (the loss of containment) in GoldSim by defining failure distributions for the barrier(s) in the packages within your Source. A package in a Source can be specified to have no barriers, a single barrier, or double barriers (one inside the other).

For a particular barrier, multiple *failure modes* can be defined, with each mode having a different failure distribution. For example, one failure mode may be assigned to represent one type of corrosion (e.g., uniform corrosion), while another may be assigned to represent another type of corrosion (e.g., pitting corrosion). GoldSim combines the failure modes in an appropriate manner to obtain the total failure distribution. It is assumed that the different modes operate independently and without synergism. Appendix E describes in detail the manner in which the separate failure modes are mathematically combined.

Read more: [Appendix E: Details of Source Computations](#) (page 399).

The figure below illustrates the combination of two failure modes.

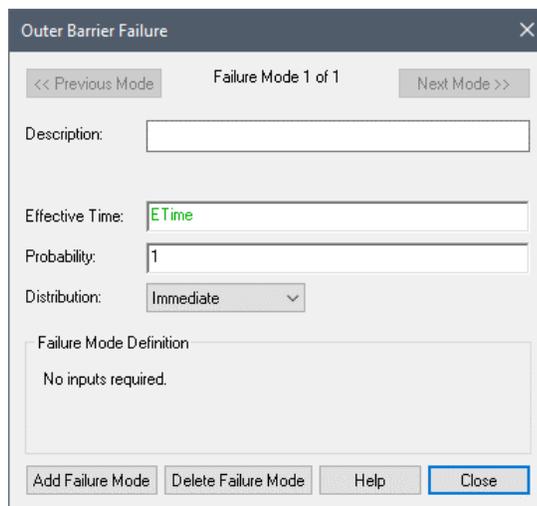


Note that within GoldSim, a barrier has only two states: unfailed or failed. The definition of “failure” is specified by the user. Typically, failure is defined as the initial breaching of the container such that material inside the barrier (i.e., contaminants) is exposed to the environment (e.g. flowing water).

## Simulating Outer Barrier Failure

If you specify the **Number of Barriers** for your Source to be either "single;" or "double", the **Outer Barrier...** button will be available on the Source dialog.

The **Outer Barrier...** button accesses the following dialog for defining the outer barrier failure modes:



Failure modes can be added and deleted using the **Add Failure Mode** and **Delete Failure Mode** buttons. You can move between existing failure modes using the **Previous Mode** and **Next Mode** buttons at the top of the dialog.

Every failure mode requires at least three inputs: the **Effective Time**, the **Probability**, and the **Distribution**:

**Effective Time:** A failure distribution is defined with respect to time (it is a frequency distribution in time). The Effective Time provides a mechanism by which you can dynamically delay, speed up, or slow down the failure rate. The default value is the elapsed time (Etime), which implies that the failure distribution starts at the beginning of the simulation and is not modified during the simulation in any way.

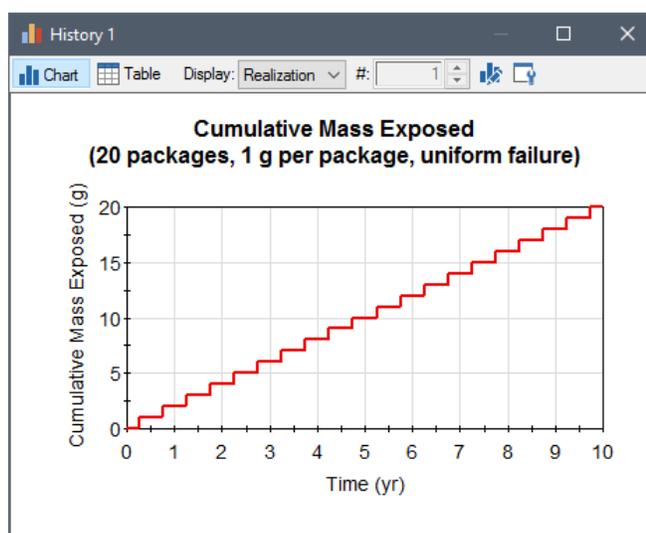
**Read more:** [Using the Effective Time to Delay/Modify Failure Distributions](#) (page 275).

**Probability:** This is the probability that the mode is active for a given package (i.e., only a small number of the packages may be susceptible to a particular failure mode). For example, while all packages may be vulnerable to uniform corrosion, only a small percentage may be vulnerable to a failure mode associated with faulty construction (e.g., bad welds). Put another way, if a barrier had only a single failure mode which had a probability of 0.5, by the end of the simulation, only 50% of the packages would have failed. The default probability for a failure mode is 1 (all packages are susceptible). Note that the probability should not be specified as a function of time (if it is, its initial value will be used).

**Distribution:** This is a list box with five options: Uniform, Weibull, Exponential, User-Defined, and Immediate. These define the shape of the failure distribution. Each type of failure distribution requires some parameters (e.g., a Uniform requires one parameter, a Weibull requires two, etc.). These additional inputs appear in the box directly below the Distribution field labeled "Failure Mode Definition".

**Read more:** [Specifying Failure Distributions for Barriers](#) (page 277).

One very important point to note regarding the Outer barrier is that *package failure is discretized*. That is, GoldSim fails packages discretely and does not fail fractional packages. Hence, if you defined a uniform failure distribution over 10 years (i.e., the packages fail at a uniform rate), and there were only 20 packages in your Source, the cumulative amount of mass exposed at the Source would look like this:



The line is jagged because the packages fail discretely.

**Read more:** [Controlling the Outer Barrier Failure Algorithm](#) (page 280).



**Warning:** If you run a Deterministic (rather than probabilistic) simulation, the package failures will not follow the specified distribution. Rather, they will all fail at the same time (the expected value of the distribution).

### ***Using the Effective Time to Delay/Modify Failure Distributions***

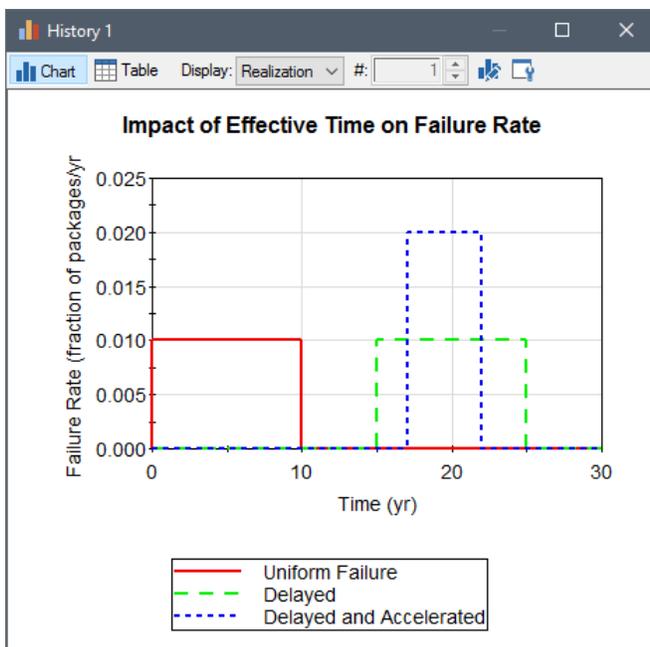
Failure distributions are frequency distributions in time. That is, they define the failure rate as a function of time. You define the shape of the distribution using one or more parameters (e.g., the uniform distribution requires a duration).

Note, however, that the parameters defining the container failure distributions cannot vary with time (i.e., a parameter that defines a distribution in time cannot vary with time). As a result, it is not possible for the failure rates to respond directly to time-varying conditions. That is, the failure distribution for a given mode must be defined *assuming a given set of conditions*. Any temporal changes in conditions (e.g., temperature, water saturation) that may affect the failure distribution must be known prior to its specification and indirectly incorporated into the form of the distribution.

The **Effective Time**, however, can be used to delay or modify failure distributions such that they can dynamically respond to time-varying conditions. For example, the failure rate could be specified to increase with increases in temperature or aggressive chemical conditions. The Effective Time represents the failure mode's view of how far along the time axis it is *relative to the start-time of the defined failure distribution*.

Hence, if the Effective Time increases faster than the elapsed time, this has the effect of accelerating failures (relative to that defined by the distribution); if the Effective Time increases at a slower rate than the elapsed time, this has the effect of decelerating failures. If the Effective Time temporarily does not increase at all as the elapsed time increases, this has the impact of temporarily stopping failures.

It is easiest to illustrate the use and physical significance of the Effective Time by considering an example. Suppose that we start with a failure distribution for a Source which is defined such that the packages fail uniformly over 10 years. Let's now consider two modifications to this distribution. In the first case, we wish to delay the start of failure by 15 years. In the second case, we wish to delay the start by 17 years, but once the distribution starts, we want the containers to fail at twice the rate. These three cases are illustrated graphically below:



Within GoldSim, we could achieve all three of these behaviors by defining a uniform failure distribution and specifying the Effective Time as follows:

Case	Effective Time
uniform failure beginning immediately	Etime
uniform failure, start delayed by 15 years	Etime-15yrs
uniform failure, start delayed by 17 years, accelerated after start by factor of 2	2 * (Etime - 17yrs)

Note that the default value for the Effective time is the elapsed time (Etime), which implies that the failure distribution starts at the beginning of the simulation and is not modified during the simulation in any way.

### Simulating Inner Barrier Failure

Whereas the outer barrier failure distribution is applied to a specified number of packages which are present in the Source, the inner barrier failure distribution is applied to each individual package. That is, it represents the failure distribution of the inner barrier(s) within a given package. One very important implication is that unlike the outer barrier, *failure of the inner barrier is not discretized*. That is, you do not specify the number of inner containers within each package. Hence, if your conceptual model is that a single inner container exists in each package (e.g., a liner within a drum), the failure distribution represents the *fraction* of the single inner container which has failed as a function of time. If your conceptual model is that multiple inner containers exist in each package (e.g., multiple drums within a large concrete container), the failure distribution represents the fraction of the inner containers which have failed as a function of time. In either case, the key point is that the fraction does not necessarily represent an integer number of inner containers.

If you specify the **Number of Barriers** for your Source to be "double", the **Inner Barrier...** button will be available on the Source dialog. The **Inner**

**Barrier...** button accesses the following dialog for defining the inner barrier failure modes:

Failure modes can be added and deleted using the **Add Failure Mode** and **Delete Failure Mode** buttons. You can move between existing failure modes using the **Previous Mode** and **Next Mode** buttons at the top of the dialog.

The behavior of the failure distribution is controlled by the following inputs:

**Start when outer barrier fails?:** If this box is checked, the failure distribution will not begin until the outer barrier fails. Otherwise, the failure distribution begins at the specified **Start Time**.

**Start Time:** Unlike the outer barrier failure distributions, which are defined relative to the Effective Time for the failure mode, inner barrier failure distributions are defined relative to a specific start time. That is, you directly specify the time at which the failure distribution begins (i.e., whether or not it is delayed). If **Start when outer barrier fails?** is checked, the beginning of the inner barrier failure distribution is controlled by the time of the failure of the outer barrier (and the **Start Time** is ignored). Otherwise, the failure distribution begins at the elapsed time specified in this field.

**Probability:** This is the probability that the mode is active for a given portion of an inner container. The default probability for a failure mode is 1 (all parts of the inner container are susceptible). Note that the probability should not be specified as a function of time (if it is, its initial value will be used).

**Distribution:** This is a list box with six options: Uniform, Weibull, Exponential, User-Defined, Immediate and Table. These define the shape of the failure distribution. Each type of failure distribution requires some number of parameters (e.g., a Uniform requires one, a Weibull requires two). These additional inputs appear in the box directly below the Distribution field labeled "Failure Mode Definition".

**Read more:** [Specifying Failure Distributions for Barriers](#) (page 277).

## Specifying Failure Distributions for Barriers

For both outer and inner barrier failure, there are six possible failure distributions that can be specified:

- Uniform;
- Weibull;

- Exponential;
- User-Defined;
- Immediate; and
- Table.

These six distribution types are described below. The mathematical details of these distributions are presented in Appendix E.

**Read more:** [Appendix E: Details of Source Computations](#) (page 399).



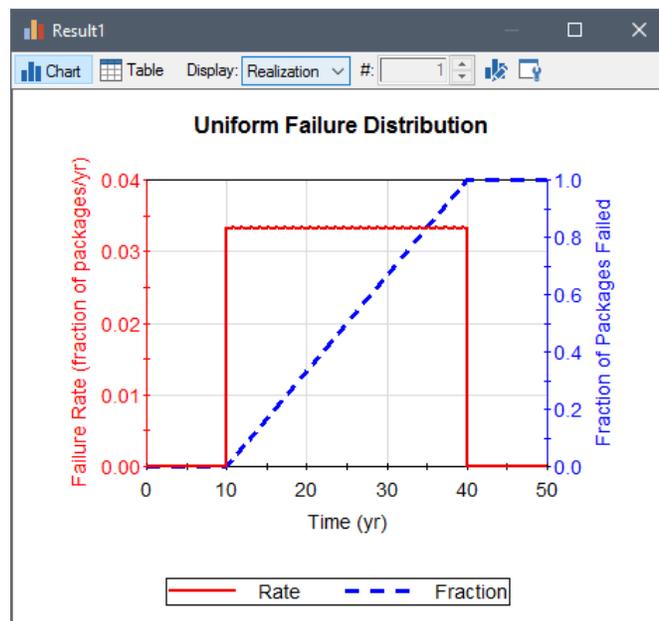
**Note:** For all of the distributions (except the User-Defined), the parameters describing them should not be specified as functions of time (if they are, only the initial values will be used).

**Immediate Barrier Failure**

The immediate distribution requires no parameters. In an immediate distribution, all containers fail immediately when the distribution begins (i.e., when the Effective Time is equal to zero).

**Uniform Barrier Failure**

A uniform failure distribution requires a single argument: the **Duration**. The Duration has dimensions of time, and represents the period over which the containers fail (at a uniform rate). The following plot is for a uniform failure distribution with a duration of 30 years that has been delayed by 10 years:



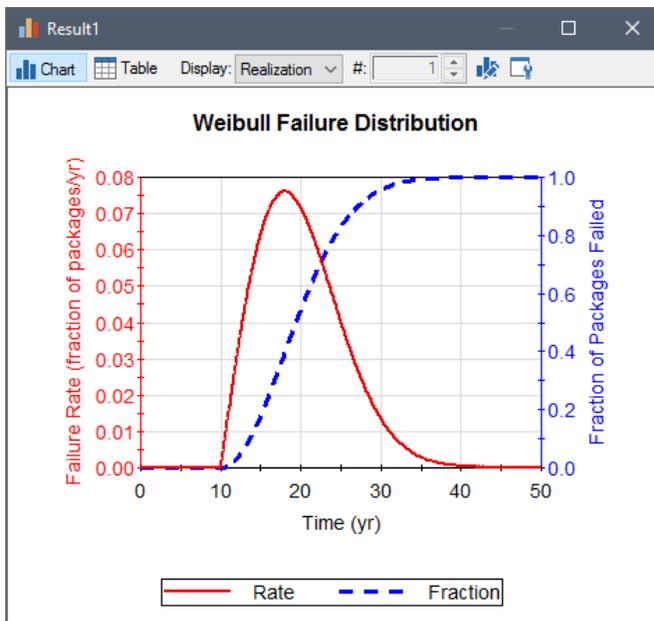
**Note:** The Duration should not be specified as a function of time. If it is, only the initial value will be used.

**Weibull Barrier Failure**

A Weibull failure distribution is often used to characterize failure times in reliability models. It has two parameters: a **Slope** and a **Mean Lifetime**. The slope is dimensionless and the mean lifetime has dimensions of time. The slope controls the shape of the distribution. A slope of 1 produces an exponential curve; a slope of 3.3 produces a normal distribution; slopes between 1 and 3.3

produce normal-like curves with a trailing tail (see below); slopes greater than 3.3 produce normal-like curves with a leading tail.

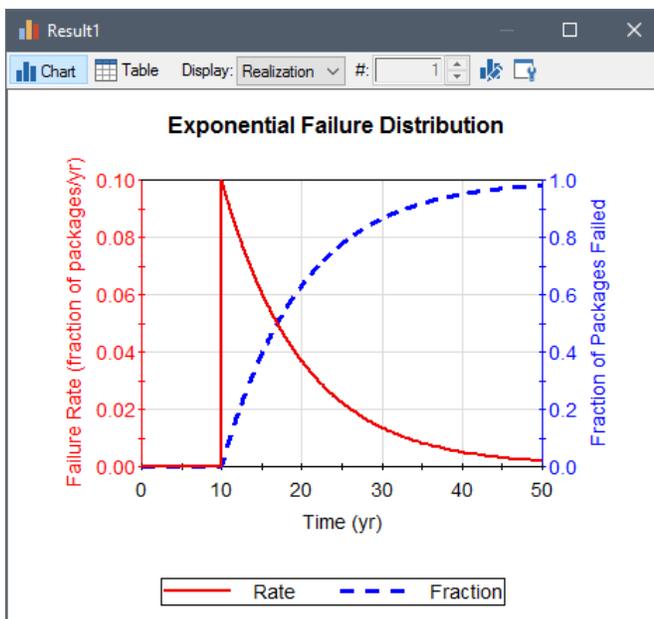
The curve below shows a Weibull distribution that has been delayed by 10 years:



**Note:** The Slope and Mean Lifetime should not be specified as functions of time. If they are, only the initial values will be used.

### Exponential Barrier Failure

An exponential failure distribution requires a single argument: the **Expected Lifetime**. The Expected Lifetime has dimensions of time, and represents the mean lifetime of a container. The curve below shows an exponential distribution that has been delayed by 10 years:





**Note:** The Expected Lifetime should not be specified as a function of time. If it is, only the initial value will be used.

---

### **User-Defined Barrier Failure**

The user-defined distribution allows the user to directly specify a custom distribution of any form, which is computed dynamically during the simulation. To define the failure distribution, you specify the **Fraction Failed** (as an expression or a link.)

The **Fraction Failed** should be specified as a dimensionless value. Typically, it will be specified as a function of the elapsed time (Etime). It should always be greater than or equal to 0 and less than or equal to 1, and can never decrease as a function of time.



**Note:** The **Effective Time** (for outer barrier failure modes) and the **Start Time** (for inner barrier failure modes) is grayed out for user-defined distributions, and any delays or modifications should be directly incorporated into the definition of the **Fraction Failed**.

---

When a user-defined distribution is used for an inner barrier failure mode which is linked to the outer barrier, the distribution is computed and saved *starting from the beginning of the simulation*, and then used at the appropriate time. For example, suppose that the user-defined distribution was specified as a function of Etime such that the inner barrier(s) failed in such a way that the **Fraction Failed** was equal to 1 at Etime = 10 years. Suppose further that the inner barrier failure was linked to the outer barrier failure, and the outer barrier failed instantaneously at 25 years. In this case, GoldSim would compute and save the failure distribution, but not apply it until 25 years (i.e., Fraction Failed would be equal to 0 at 25 years, and 1 at 35 years).

### **Table Barrier Failure**

In some cases, rather than entering a custom failure distribution by directly specifying the Fraction Failed, you may wish to use an external function to specify the custom failure distribution. This may be useful, for example, if the failure distribution is relatively complex and varies from realization to realization.

To facilitate this, GoldSim allows you to define a failure distribution by entering a link representing a 1-D **Table Definition**. As discussed in detail in the **GoldSim User's Guide** (in a section entitled "Using an External Element to Define Look-Up Tables"), External elements can produce special outputs representing look-up tables.

The **Table Definition** for a failure mode must be a 1-D Table Definition output produced by an External element. The independent variable for the table must have dimensions of time (which represents the Effective Time for the failure distribution), and the dependent variable must be dimensionless. In addition, the dependent variable for the table should must be greater than or equal to 0 and less than or equal to 1, and can never decrease as a function of time.

Note that if the table terminates at a Fraction Failed which is less than 1, GoldSim does not extrapolate the table (i.e., barrier failure is assumed to stop).

### **Controlling the Outer Barrier Failure Algorithm**

You can control the manner in which GoldSim discretizes outer barrier failures in two ways. Both of these options are located in the **Contaminant Transport** tab of the Options dialog (accessed via **Model | Options...**):

The screenshot shows the 'Options' dialog box with the 'Contaminant Transport' tab selected. Under 'General Options', 'Solution precision' is 'Medium (default)', 'Log warning messages' is checked, 'Log cell-network details' is unchecked, and 'Disable decay of species' is unchecked. Under 'Source Term', 'Barrier failure type' is 'Random failure time' and 'Round (vs truncate) the computed number of waste-package failures' is checked. Under 'Display Units', 'Mass in pathways' is 'g (M)', 'Mass fluxes' is 'g/yr (M/T)', 'Fluid concentrations' is 'mg/l (M/L3)', and 'Solid concentrations' is 'g/kg (M/M)'. There is a 'Restore defaults' button and 'OK', 'Cancel', and 'Help' buttons at the bottom.

The two options in the "Source" section can be used to control the manner in which GoldSim discretizes outer barrier failure.

**Barrier failure type:** This is a list box with two options: "Predicted failure time" (the default), and "Random failure time".

If "Predicted failure time" is selected, package failures are discretized by computing the cumulative fraction failed based on the distribution, multiplying this fraction by the total number of packages, and truncating or rounding (see below) to the nearest integer number of packages. As a result, multiple realizations of the same failure distribution will be identical.

If "Random failure time" is selected, the failure time for each package is randomly sampled from the distribution. As a result, multiple realizations of the same failure distribution will be slightly different.



**Note:** The Random failure time option can not be applied to user-defined distributions. These distributions are always computed based on predicted failure times.

**Round (vs truncate) the computed number of waste-package failures:** This checkbox determines how package failure is discretized (and only applies if "Predicted failure time" is selected under **Barrier failure type**). It is best explained using an example. Suppose you had 10 packages that failed uniformly over 10 years. If this box was checked, the first package would fail at 0.5 years, and the last package would fail at 9.5 years. If this box was cleared, the first package would fail at 1 year, and the last package would fail at 10 years.

## Disrupting Packages Using Discrete Events

In addition to failing packages by defining failure distributions, you can also fail packages via discrete events.

The field **# Packages failed by events** accepts discrete change signals (produced, for example, by a Discrete Change element). Discrete change signals

are discussed in detail in "Simulating Discrete Events" in the **GoldSim User's Guide**. Discrete change signals have associated with them an *instruction*, which can be Add or Replace.



**Note:** If no barriers are specified (i.e., **Number of Barriers** is specified as “none”), the **# Packages failed by events** field is grayed out, since it is not applicable in this case.

This field only accepts discrete change signals which are dimensionless and positive, and have associated with them an Add instruction (Replace instructions are not permitted and will result in a run-time error). Multiple signals can be specified by separating the various entries with a semi-colon.

When a signal is received by the Source, the specified number of packages is instantaneously disrupted (both outer and inner barriers are failed). When packages are failed, the number of unfailed packages is automatically adjusted accordingly (i.e., GoldSim treats this discrete change like another failure mode.)

## Source Outputs

Sources have at least three outputs:

- **Failed\_Packages.** This is the number of failed packages in the Source, and is dimensionless.
- **Unexposed\_Mass.** This is a vector by species with dimensions of mass. It represents the mass of each species in the Source which is unexposed (i.e., still within unfailed barriers or undegraded matrix).

In addition, for every Inventory Cell specified, an output is created on the Source:

- **Cumulative\_to\_Cell**, where *Cell* is the name of the Inventory Cell. This is a vector by species, and has dimensions of mass. It represents the cumulative amount of mass of each species which has been exposed and placed into the Cell.

Note that this output is automatically linked into the Cumulative Input field for the associated Inventory Cell (and cannot be edited):



The *Cumulative\_to\_Cell* output of the Source element is linked into the Cumulative Input field in the input dialog for all Inventory Cells

## Instantaneously Moving Mass from a Source

In some situations, you may wish to instantaneously move mass from a Source (e.g., a consequence of a disruptive event of some sort). This can be accomplished in two ways:

- **Moving mass from an Associated Cell:** You could *decrement* the mass in an Associated Cell by specifying a negative Discrete Change. You could then *increment* the mass in a Cell at some other location in

the system by the same amount in order to represent the discrete movement of the mass. For example, you could move half of the exposed mass in one associated Cell to another Cell on the ground surface.

**Read more:** [Simulating Discrete Changes to the Mass Inventory in a Cell](#) (page 132).

- **Moving Unexposed Mass in a Source:** By referencing the "Unexposed\_Mass" output, you could *increment* the amount of mass in a Cell at some other location in your system by some fraction of the amount of unexposed mass in the Source. Note, however, that GoldSim does not provide a way for you to discretely decrement the amount of unexposed mass. Hence, this approach should only be used if the fraction of unexposed mass being moved is small relative to the total amount of unexposed mass (otherwise, you will create mass in your system).

## Source Example Models

The two simple examples below provide an introduction to the kinds of problems that can be solved using Sources.

### Source Example #1: Barrier Failure and Solubility-Controlled Release

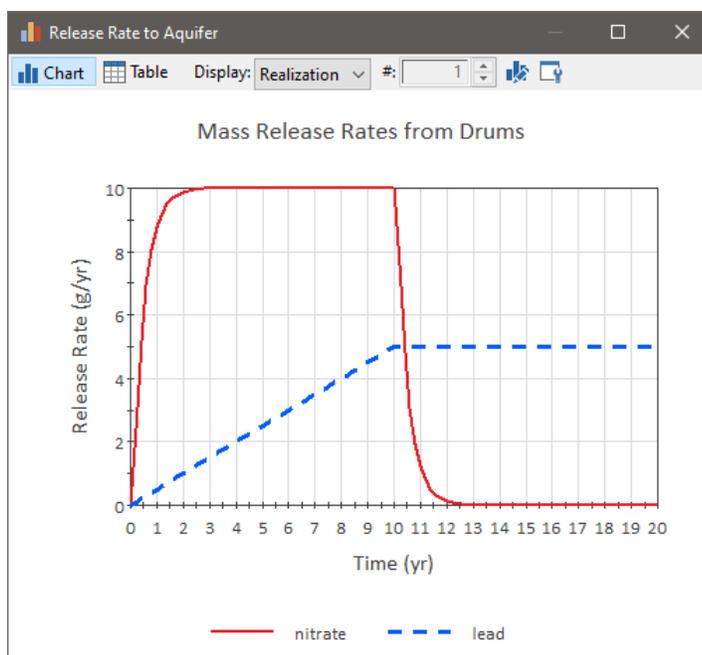
This particular example file, Source1\_Barriers.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

Suppose that 100 drums were buried in shallow soil. The soil recharges a shallow aquifer. Each drum contains water (55 gallons) and two contaminants: 1 gram of nitrate and 1 gram of lead. Nitrate is very soluble, and hence is completely dissolved in the water within the drum. The lead, however, has a solubility of 0.1 mg/l. The drums are expected to fail at a uniform rate over 10 years. Once they fail, infiltrating water flows through each drum at a rate of 0.5 m<sup>3</sup>/yr. For simplicity, we can assume that neither species sorbs onto the surrounding soil once it is released. At what rate does the mass of the two species enter the aquifer?

To simulate this system in GoldSim, you would do the following:

1. Define two species (nitrate and lead);
2. Define the properties for the medium Water (in particular, the solubility of lead in Water);
3. Define a Source, and specify the number of packages, the inventory of each species in the Source, and the failure rate of the packages;
4. Define a Cell (representing the interior of a single drum). It will automatically be assigned as an Inventory Cell for the Source;
5. Define a Cell representing the aquifer (used here simply as a sink); and
6. Specify the simulation settings (i.e., duration and timestep), and run the model.

The output of this simulation, in the form of time histories of the mass flux of each species from the drums into the aquifer, is shown below:



Note that the nitrate species is released uniformly over 10 years as the drums fail and it is flushed into the aquifer (the rounded front and back of the curve are due to the finite amount of time it takes to flush a drum). The lead species, on the other hand, is controlled by a solubility constraint within each drum. That is, the release rate from a given failed drum is constant. The release rate from the Source increases linearly as more drums fail. After all the drums have failed, the release rate stays constant (and will continue to do so until all of the lead has dissolved).



**Note:** Because this example includes a Source element, it requires the RT Module. If you are using the CT Module, you will not be able to open the file.

## Source Example #2: Matrix Degradation

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4).

To illustrate how matrix degradation is simulated, we will consider a simple example. This particular example file, Source2\_MatrixDegradation.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

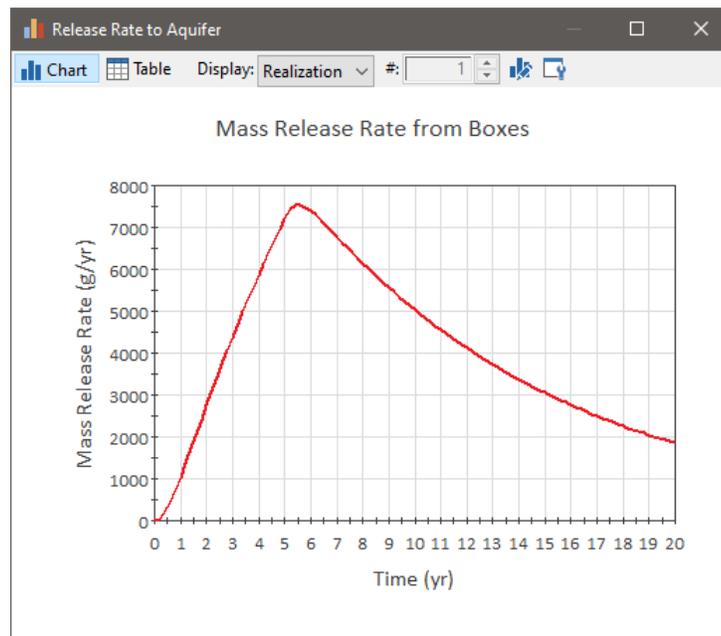
Suppose that 100 steel boxes were buried in shallow soil. Rainfall infiltrating through the soil recharges a shallow aquifer. Each box contains grouted waste containing 10 grams of a soluble contaminant. The boxes are expected to fail at a uniform rate over 5 years. Once they fail, infiltrating water will flow through each box at a rate of  $0.5 \text{ m}^3/\text{yr}$ . The grout, however, degrades very slowly (1% per year). For simplicity, we can assume that the species does not sorb onto the surrounding soil once it is released. At what rate does the contaminant mass enter the aquifer?

To simulate this system in GoldSim, you would do the following:

1. Define the contaminant species;

2. Define a Source, and specify the number of packages, the inventory of the contaminant species in the Source, the failure rate of the packages, and the matrix degradation rate (of  $0.01 \text{ yr}^{-1}$ );
3. Define a Cell (representing the interior of a box). It will automatically be assigned as an Inventory Cell for the Source;
4. Define a Cell representing the aquifer (used here simply as a sink) link it to the Source Cell; and
5. Specify the simulation settings (i.e., duration and timestep), and run the model.

The output of this simulation, in the form of time histories of the mass release of each species from the boxes into the aquifer, is shown below:



The release rate increases almost linearly as packages fail over the first 5 years. Afterward, the release rate decreases as the matrix slowly degrades and releases mass (and at 20 years, not all of the mass has been released). Note that this part of the curve is actually exponential, since a fractional degradation rate results in an exponentially decreasing amount of mass in the Source.

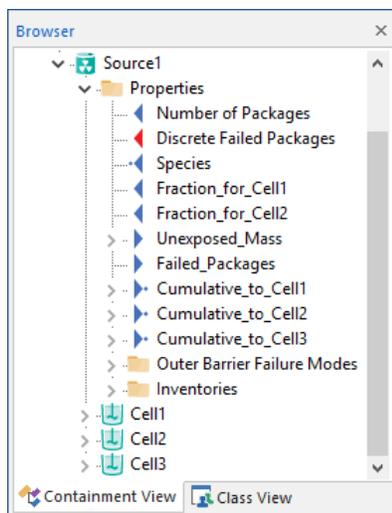


**Note:** Because this example includes a Source element, it requires the RT Module. If you are using the CT Module, you will not be able to open the file.

**Read more:** [What is the Difference Between GoldSim CT and GoldSim RT?](#) (page 4).

## Viewing a Source in the Browser

The browser view of a Source is shown below:



Because a Source is also a Container, in the browser, the contents of the Container are shown. The actual properties of the Source (the inputs and outputs) are shown within a Properties folder.



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

Within the Properties folder, the primary inputs for the Source (number of packages, Discrete failed packages, and fractions to Inventory Cells) are listed first. Note that the Species input also appears. The Species input is automatically linked to the nearest Species element when the Source is created. *This link cannot be changed using the Link Cursor, and is displayed for information purposes only.*

The Source's outputs are listed next.

Below the outputs, the inputs defining the outer barrier and inner barrier failure modes are contained in folders. Each failure mode has a separate folder. Finally, the Inventory inputs are listed in a folder.

Following the Inventory folders, the contents of the Source Container are listed.

## Saving Results for a Source

The three outputs for a Source are saved by clicking **Final Values** and/or **Time History** at the bottom of the Source editing dialog:

Save Results	Final Values	Time History
Unexposed Mass in Source:	<input type="checkbox"/>	<input type="checkbox"/>
Cumulative Releases to Inventory Cells:	<input type="checkbox"/>	<input type="checkbox"/>
Number of Failed Packages:	<input type="checkbox"/>	<input type="checkbox"/>

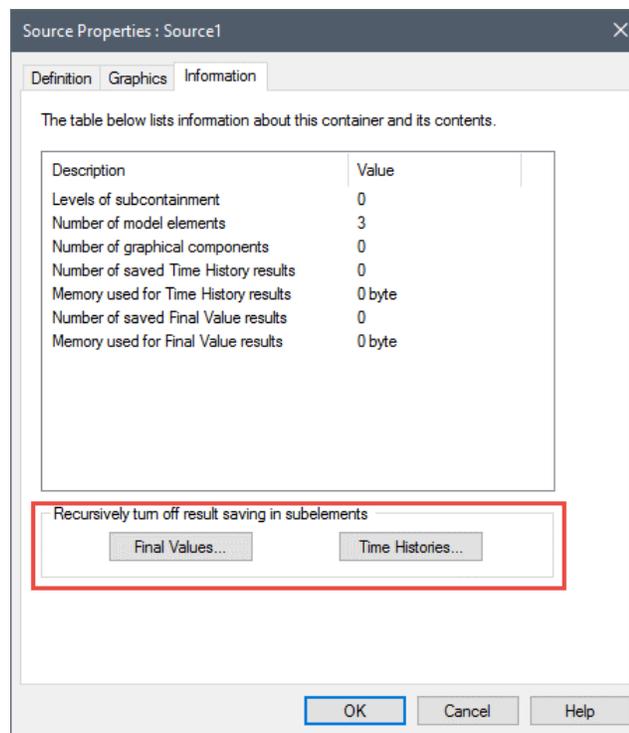
If you are running multiple realizations, the Time History box is ignored, and unless an output is connected to a Time History Result element, no time history results will be saved. In fact, in such a case, the Save Results section would look like this:

Save Results	Final Values	Monte Carlo Histories
Unexposed Mass in Source:	<input type="checkbox"/>	<input type="checkbox"/>
Cumulative Releases to Inventory Cells:	<input type="checkbox"/>	<input type="checkbox"/>
Number of Failed Packages:	<input type="checkbox"/>	<input type="checkbox"/>

In this particular case, because the simulation involves multiple realizations, the “Time History” checkbox is replaced by a “Monte Carlo Histories” checkbox. This checkbox is grayed out, since it is only used for information purposes. You cannot edit it directly, and its appearance is completely determined by whether or not the output is connected to a Time History Result element. That is, in order to save time history results for a Source output when running multiple realizations, you must connect it to a Time History Result element.

In some cases, you may want to disable all results for elements inside the Source.

You can do this using the two buttons located at the bottom of the **Information** tab or the Source dialog:



**Note:** The **Time Histories** button is only available if you are running a single realization. If you are running multiple realizations, the state of each element’s Time History flags are determined by whether or not the element is referenced by an active Time History Result element. If it is, the flag is turned on. If it is not, the flag is turned off. In both cases, the flag is grayed out and cannot be manually changed.

To globally turn off saving of all of the results of a particular type in a Source, simply press the button. A dialog will be displayed asking you to confirm that you wish to turn off the results.

Of course, once you turn off results in a Source, you can subsequently enter the Source and set some of the elements’ results flags back on.

By default, you cannot turn off results for outputs which are linked to Result elements (unless the Result element is a Time History Result element that has been disabled). That is, any output linked to a Result element is automatically saved even if you choose to turn off results using the buttons described above. This behavior can be changed in Time History Result elements (so the outputs linked to the Result element are not automatically saved) by disabling the element.



**Note:** For Cells inside the Source, these Global result flags for the Source Container do not impact the **Output Precipitated Mass** checkbox.

---

---

# Chapter 6: Receptors

It isn't pollution that's harming the environment. It's the impurities in our air and water that are doing it.

Dan Quayle

## Chapter Overview

The objective of many contaminant transport studies is to compute not only contaminant concentrations or flux rates at various locations in the environment, but also the impact of these contaminants on specific receptors (e.g., humans, wildlife, flora).

GoldSim can calculate impacts in terms of health risks, doses; or hazard indexes.

The GoldSim Contaminant Transport module contains a special element referred to as a *Receptor* to facilitate this. This short chapter describes the specification and use of Receptors in GoldSim.

### In this Chapter

This chapter discusses the following:

- Computing Impacts to Receptors
- Defining a Receptor
- Viewing a Receptor in the Browser
- Saving Results for a Receptor

## Computing Impacts to Receptors

The impact to a receptor (e.g., a farmer) from being exposed to contaminants via a particular pathway (e.g., by ingesting contaminated water) is typically computed by multiplying contaminant concentrations in an environmental medium (e.g., water, soil, blood) to which the receptor is exposed by user-defined *impact conversion factors*.

Impacts are quantified either as an incremental cancer risk per individual per unit time, a radiation dose per unit time, or a Hazard Index (the concentration in a medium divided by a reference concentration).

The *total impact* to a receptor is computed as the sum of the impacts associated with each pathway through which the receptor is exposed to the contaminant (e.g., drinking water from a well, breathing dust in the atmosphere, ingesting soil).

Impact conversion factors are species- and receptor-specific and have dimensions of impact per unit concentration.

Within GoldSim, you usually compute an impact by using a Receptor element to carry out a term-by-term multiplication of the species concentration vectors from media in pathways by vectors of impact conversion factors. The result would be an impact vector. It is a vector because it contains an item for each species.

As described in "Using Vectors and Matrices" in the **GoldSim User's Guide**, you can carry out a term-by-term multiplication of two vectors using the multiplication (\*) operator:

Impact = Concentration\_Vector \* Impact\_Conversion\_Factor\_Vector

Typically, the impact to a receptor will be a sum of several term-by-term vector multiplications, since the receptor is likely to interact with multiple contaminated media (e.g., water in a well, soil, dust).



**Note:** Once you have an impact vector, you could compute a total impact (summed over all species) by using the **Sumv** function. As discussed in "Using Vectors and Matrices" in the **GoldSim User's Guide**, the **Sumv** function sums the components of a vector (producing a scalar)

---

## Defining a Receptor

Although you could compute impacts by simply using an Expression element, for convenience, the Contaminant Transport Module provides a specialized version of an Expression element called a Receptor to facilitate this calculation.

The dialog for a Receptor is shown below:

The dialog has three inputs:

**Impact type:** This is the type of impact to be computed. GoldSim provides three options:

- Risk (e.g., health or cancer risk);
- Dose (radioactive dose); and
- Hazard Index.

The choice of the **Impact type** determines the dimensions of the Receptor output (and therefore the dimensions of the vector accepted by the **Impact** input field):

- A Risk has dimensions of inverse time (e.g., the incremental cancer risk per individual per year);
- A Dose has dimensions of radiation dose per time (e.g., mrem/yr, Sv/yr);
- A Hazard Index is dimensionless and is intended to represent a ratio of concentrations (the concentration in a medium divided by some reference concentration).

**Impact:** This is the equation describing the impact itself. It must be a vector by species. Its dimensions are determined by the impact type.

For Risk and Dose impacts, it will typically be specified as a sum of several term-by-term vector multiplications (a concentration vector multiplied by an impact conversion factor vector).

For a Hazard Index impact, it will typically be specified as a sum of several term-by-term vector divisions (a ratio of concentrations).

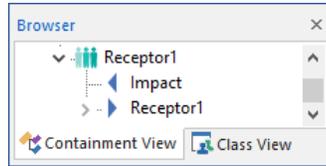
The multiplication (\*) and division (/) operators can be used to carry out a term-by-term multiplication or division of two vectors. This is discussed in "Using Vectors and Matrices" in the **GoldSim User's Guide**.

**Display Units:** This is the units in which the output of the Receptor is displayed. The acceptable dimensions are determined by the Impact Type

(inverse time for Risk, dose/time for Dose, dimensionless for Hazard Index).

## Viewing a Receptor in the Browser

The browser view of a Receptor is shown below:



**Note:** Element inputs and outputs are only shown in the browser if you choose to **Show element subitems** (accessed via the browser context menu by right-clicking in the browser).

As can be seen, in the browser, a Receptor has a single input (the Impact equation), and a single output (the resulting impact vector).

## Saving Results for a Receptor

Receptors have a single output, the resulting impact vector. It is a vector by species, and its dimensions are defined by the impact type.

You specify that you wish to save these results by clicking **Final Values** and/or **Time History** at the bottom of the Receptor editing dialog:

Save Results \_\_\_\_\_  
 Final Values     Time History

If you are running multiple realizations, the Time History box is ignored, and unless an output of the element is connected to a Time History Result element, no time history results will be saved at all for the element. In fact, in such a case, the Save Results section (for items 1 and 3 above) would look like this:

Save Results \_\_\_\_\_  
 Final Values     Monte Carlo Histories

In this particular case, because the simulation involves multiple realizations, the “Time History” checkbox is replaced by a “Monte Carlo Histories” checkbox. This checkbox is grayed out, since it is only used for information purposes. You cannot edit it directly, and its appearance is completely determined by whether or not the output is connected to a Time History Result element. That is, in order to save time history results for a Receptor when running multiple realizations, you must connect it to a Time History Result element.

---

# Chapter 7: Advanced Modeling Concepts

A child of five would understand this.  
Send someone to fetch a child of five.

Groucho Marx

## Chapter Overview

This chapter discusses a number of advanced contaminant transport modeling issues, and how GoldSim can be applied to them. It will primarily be of interest to experienced contaminant transport modelers.

### In this Chapter

In particular, this chapter includes discussions of the following topics:

- Representing Spatial Variability
- Non-Linear Partitioning
- Modeling Complex Chemical Reactions
- Simulating Non-Chemical Constituents

## Representing Spatial Variability

All real environmental systems are variable to some extent. For example, aquifers are generally heterogeneous with respect to flow and transport properties, chemical conditions vary spatially throughout the environment, and flow rates vary spatially within a stream. Such variability can have a large influence on the behavior of the system, and it is therefore very important to represent this in your model.

Much of this variability can be directly represented within GoldSim using the basic structure and features of transport pathways and sources. For example, variability in transport pathways can be represented by defining multiple pathways with differing properties, and barrier failure distributions in contaminant sources typically reflect spatial variability in chemical and/or hydrologic conditions.

How would one represent, however, the fact that the decay rate or partition coefficient for a contaminant is spatially variable? In this case, the solution is to define separate Solid, Fluid or Species elements in each location where the properties vary.

### Defining Spatially Variable Decay Rates

In general, the properties of a Species element must, by definition, be constant throughout your model (e.g., you would not want the Molecular Weight of a Species to take on different values in different locations in your model). As a result, when you create a model using the Contaminant Transport Module, a single Species element is automatically created. This element can be moved, but cannot be deleted. Moreover, GoldSim does not allow you to insert additional Species elements.

There are, however, two Species element properties, the Decay Rate and the associated Stoichiometries, that you occasionally may wish to take on different values at different locations in your model. For example, you may want a species to decay only in certain pathways (e.g., a pathway representing anoxic sediments; or a pathway representing the liver in a pharmacokinetic model).

Because pathway and Source elements automatically link to the Species element, and the Decay Rate and Stoichiometries are properties of the Species element, the only way to allow these inputs to have different values in different pathways (or Sources) is to create multiple Species elements (with different Decay Rates and/or Stoichiometries) in different Containers such that different pathways (and Sources) link to different Species elements. As pointed out above, however, GoldSim does not allow you to *insert* additional Species elements. You can, however, create *clones* of the Species element, and this allows you to accomplish exactly what is outlined above.



**Note:** In order to understand how to spatially vary the Decay Rate or Stoichiometries in your model, you must be comfortable with cloning elements and localizing Containers. Both of these topics are discussed in Chapter 10 of the **GoldSim User's Guide**.

---

Cloned elements automatically mimic each other, such that if you change a property of a clone, the property is automatically changed in all of the other clones. Hence, cloning a Species element does not create inconsistencies in your model, since if you change a property (such as the Atomic Weight) in one clone, it is automatically changed in all the other clones. How, then, can you use a clone to vary the Decay Rate or Stoichiometries in different clone species?

This can be accomplished because you can enter a link (a reference to another element's output), rather than just entering a number when defining a Decay Rate or a Stoichiometry. If you enter a link ID into an input field for a clone element, the same ID will appear in the corresponding input field of all of the clone elements. If, however, different elements having that same ID exist at the locations (Containers) where the clones are, each clone will link to a different element defining the Decay Rate or Stoichiometry, allowing that parameter to be different in each Container.

### **Procedure for Defining Spatially Variable Decay Rates**

The steps required to create a spatially variable Decay Rate are outlined below. The procedure would be identical for creating spatially variable Stoichiometries.

1. Identify the pathway(s) and/or Source(s) which will utilize spatially variable decay rates.
2. Localize the Containers that those pathways/Sources are located in.
3. Create a clone of the Species element in each of those localized Containers. (Note that unlike most other elements in GoldSim, all clones of the Species element are forced to have the same ID. As a result, Species clones must be placed in localized Containers).
4. Insert elements defining the spatially variable decay rates in each localized Container, and link them to each local Species clone. Note that these elements must have the same name (since they are referenced by a cloned Species element), but they themselves should *not* be clones.

### **Defining Spatially Variable Media Properties**

In many cases, you will want the properties of the environmental media in your model to vary spatially. For example, the solubility for a species in Water or the partition coefficient for a species in Sand may take on different values in different locations (pathways) in your model.

The simplest way to accommodate this is to simply have pathways and Sources reference different media at different locations in your model. This approach will work well for Solids and most Fluids.

Note, however, that there can be only one Reference Fluid in your model, and like the Species element, it cannot be copied. Hence, if solubility or one of the other Reference Fluid properties varies spatially in your model (e.g., due to a change in pH along a flow path), you cannot represent this simply by copying or inserting multiple Reference Fluids in different portions of your model.

GoldSim provides two ways to vary the properties of the Reference Fluid:

1. You can create a new Fluid (by defining new Fluids with a set of Solubilities rather than a set of partition coefficients); or
2. You can create a clone of the Reference Fluid.

The resulting behavior of the system using these two approaches has some important differences, which are outlined below. The manner which you select will be a function of which of these two approaches best represents the actual behavior of the system you wish to simulate.

### **Using Multiple Fluids to Represent Spatially Variable Fluid Properties**

One way to represent spatially variable properties of a Fluid (such as water) is to simply create multiple fluids. For example, if the pH varied significantly between two locations, then the solubilities may also change significantly. To represent this, you could simply create a second fluid (e.g., High\_pH\_Water), and assign it a different set of solubilities. You could then place the Reference Fluid (e.g., Water) in Cells in one portion of your model, and High\_pH\_Water in the other Cells, as appropriate.

When you create a Fluid and assign it a set of solubilities (instead of partition coefficients), GoldSim automatically computes the partition coefficients as the ratio of the solubilities in the Fluid to the solubilities in the Reference Fluid.

**Read more:** [Defining Fluids](#) (page 69).

---



**Warning:** If you choose to specify solubilities (rather than partition coefficients) for a Fluid, and the Reference Fluid has unlimited (negative) solubilities for some of the species, you must also specify unlimited (negative) solubilities for the same species (and only those species) in the Fluid. If there is an inconsistency in specifying the solubilities (i.e., unlimited solubilities in one fluid but defined solubilities in another), GoldSim will produce a fatal error message when you try to run the model.

---

### **Cloning the Reference Fluid to Represent Spatially Variable Fluid Properties**

To better understand the implications of simulating spatially variable fluid properties in this manner, it is instructive to consider a situation in which two Cells with different fluids (having different solubilities) are connected by a diffusive mass flux link. Let us further assume that a very large amount of species mass is added to one of the Cells (such that both Cells must eventually be saturated). If we run such a simulation long enough, the system will eventually reach a steady state. *At steady state (the time at which there is no net flux between the cells), if one Cell is at the solubility limit, then both Cells must be at their solubility limit. As a result, a concentration gradient will exist between the two Cells (since the solubilities are different).*

Another way to represent spatially variable properties of a Fluid (such as water) is to clone the Reference Fluid. For example, if the pH varied significantly between two locations, then the solubilities may also change significantly. To represent this, you could clone the Reference Fluid and assign it a different set of solubilities. You could then place the different clones of the Reference Fluid in different portions (Containers) of the model, as appropriate.

In order to understand how to clone the Reference Fluid (and other media elements), you must be comfortable with cloning elements and localizing Containers. Both of these topics are discussed in Chapter 10 of the **GoldSim User's Guide**. Clone elements automatically mimic each other, such that if you change a property of a clone, the property is automatically changed in all of the other clones. Hence, if you clone the Reference Fluid element and change a property (such as a solubility) in one clone, it is automatically changed in all the other clones.

How, then, can you use a clone to vary a property (such as the solubility) in a different clone medium? This can be accomplished because if you enter a link ID into an input field for a clone element, the same ID will appear in the corresponding input field of all of the clone elements. If, however, different elements having that same ID exist at the locations (Containers) where the clones are, each clone will link to a *different* element for that particular input, allowing the value of the property to be different in each Container.

The steps required to create a cloned spatially variable fluid are outlined below:

1. Make sure that the fluid properties that you wish to be spatially variable are defined via links (i.e., an element ID).
2. Identify the pathway(s) and/or Source(s) which will utilize spatially variable media properties.
3. Localize the Containers that those pathways/Sources are located in.

4. Create a clone of the Reference Fluid in each of those localized Containers.
5. Insert elements defining the spatially variable properties in each localized Container, and link them to each local Reference Fluid clone. Note that these elements must have the same name (since they are referenced by a cloned media element), but they themselves should *not* be clones.

Two points should be noted when cloning the Reference Fluid:

- Unlike most other elements, when you clone the Reference Fluid, the IDs of the clones are forced to be identical. As a result, the clones must be placed in separate localized Containers.
- Unlike other fluids (in which the partition coefficient is equal to the ratio of the solubilities), *the partition coefficients between cloned Reference Fluids are automatically defined by GoldSim as being equal to one.*

To better understand the implications of simulating spatially variable fluid properties in this manner, it is instructive to consider a situation in which two Cells (necessarily present in two different Containers) with cloned Reference Fluids (having different solubilities) are connected by a diffusive mass flux link. Let us further assume that a large amount of species mass is added to one of the Cells (such that the Cell with the lowest solubility must eventually be saturated). If we run such a simulation long enough, the system will eventually reach a steady state. *At steady state (the time at which there is no net flux between the cells), only one of the Cells will be at the solubility limit (the Cell with the lower solubility), and no concentration gradient will exist between the two Cells (the concentrations in the two Cells will be identical).*

Note that this is in contrast to the situation in which two different fluids are used (rather than a cloned Reference Fluid). In that case, the Cells will maintain a concentration gradient, and at steady state, if one Cell is saturated, the other Cell must also be saturated.

## Non-Linear Partitioning

If the partition coefficients in your model are defined as being independent of the concentration of the species (at a given temperature), the concentrations then vary linearly with mass in the Cell (assuming no solubility constraints). This relationship is referred to as a *linear isotherm*.

In many systems, however, species partition between media (e.g., water and sediment) according to a *non-linear isotherm*, in which the degree of partitioning varies with concentration. Non-linear isotherms can be readily represented in GoldSim by defining the partition coefficients as functions of the concentrations.

In many systems, species partition between media (e.g., water and sediment) according to a *non-linear isotherm*, in which the degree of partitioning varies with concentration. To illustrate the way in which you could represent non-linear partitioning, we will consider one common type of non-linear isotherm, the *Langmuir isotherm*. This particular example file, Langmuir.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).

The Langmuir isotherm is described mathematically as follows:

### Non-Linear Partitioning Example: The Langmuir Isotherm

$$c_{\text{sorbed}} = \frac{c_{\text{sorbed,max}} \cdot K_{\text{Lang}} \cdot c_{\text{diss}}}{1 + K_{\text{Lang}} \cdot c_{\text{diss}}}$$

where:

- $c_{\text{sorbed}}$  = the sorbed concentration (M/M);
- $c_{\text{sorbed,max}}$  = the maximum sorbed concentration (M/M);
- $c_{\text{diss}}$  = the dissolved concentration (M/L<sup>3</sup>); and
- $K_{\text{Lang}}$  = the Langmuir partition constant (L<sup>3</sup>/M).

This equation can be rearranged to yield an effective solid/water partition coefficient:

$$K_{\text{nl}} = \frac{c_{\text{sorbed}}}{c_{\text{diss}}} = \frac{c_{\text{sorbed,max}} \cdot K_{\text{Lang}}}{1 + K_{\text{Lang}} \cdot c_{\text{diss}}}$$

To illustrate this, consider an example in which we simulate a single Cell containing 1 m<sup>3</sup> of Water and 1kg of Sand.

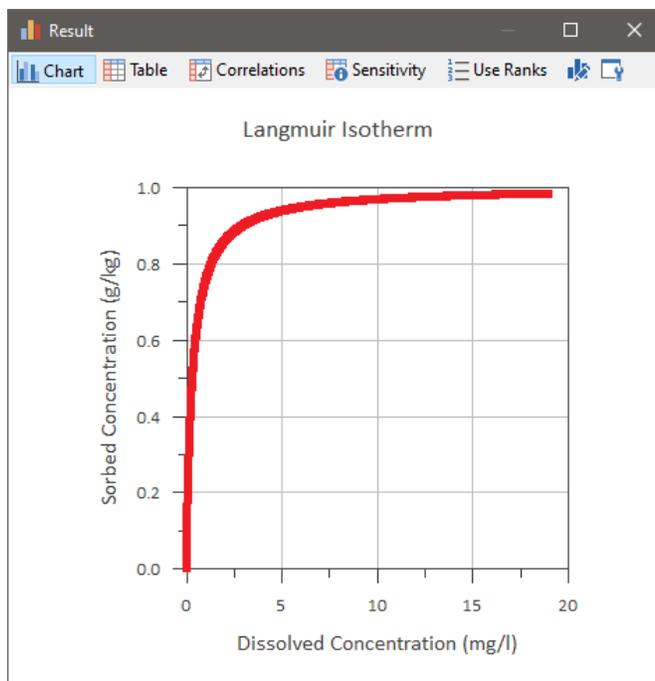
The Cell contains an initial mass of Species1. The Cell has no mass flux links; our objective is to simply plot the concentration of Species1 in the Sand as a function of the total mass in the Cell. We do this by running the simulation for multiple realizations and varying the initial mass in the Cell (a uniform distribution between 0 and 20 g). We will assume that the maximum sorbed concentration is 1 g/kg, and the Langmuir partition constant is 3 m<sup>3</sup>/kg.

To simulate this system in GoldSim, you would do the following:

1. Define a single species and two media (Water and Sand);
2. Define a single Cell containing 1 m<sup>3</sup> of Water and 1 kg of Sand;
3. Define the initial mass in the Cell as a Stochastic (a uniform between 0 and 20 g);
4. Create two constants, the maximum sorbed concentration and the Langmuir partition constant;
5. Define the partition coefficient for Species1 for the Cell using the equation specified above; and
6. Specify the simulation settings (in this case 100 realizations with 10 timesteps for 1 day) and run the model.

Note that step five creates a recursive model (since the dissolved concentration is a function of the partition coefficient, and the partition coefficient is a function of the dissolved concentration). Hence, when you do this, you must utilize a previous value element. Previous value elements are discussed in detail in Chapter 10 of the **GoldSim User's Guide**. As discussed in that section, you must take extra care when simulating systems with Previous value elements to ensure that your timestep is appropriately small.

The output of this simulation, in the form of a scatter plot of the sorbed concentration (the concentration in Sand) versus the dissolved concentration, is shown below:



For linear partitioning, this would be a straight line. As can be seen, non-linear isotherms "bend" over and approach a maximum.



**Note:** Since you can only reference the concentration in the fluid *leaving* a Pipe or Aquifer pathway, it will likely not be appropriate to use this to compute the partition coefficient throughout the entire length of the pathway. Hence, in general, non-linear partition coefficients should only be applied (i.e., defined for solids present) within Cell pathways.

## Modeling Complex Chemical Reactions

Mathematically, if A decays to B, GoldSim computes the rate of change of mass (at a particular location) as follows:

$$dM_A/dt = - M_A \lambda_A$$

$$dM_B/dt = M_A \lambda_A R_{BA} W_B / W_A$$

where:

$M_A$  = the mass of species A (mass);

$dM_A/dt$  = the rate of change of species A (mass/time);

$dM_B/dt$  = the rate of change of species B (mass/time);

$\lambda_A$  = decay rate of species A (1/time);

$R_{BA}$  = stoichiometry (moles B produced per moles A decayed);

$W_A$  = molecular (or atomic) weight of species A; and

$W_B$  = molecular (or atomic) weight of species B.

These equations are appropriate for first-order decay reactions.



**Note:** In order to model reactants, you must have the RT Module. If you are using the CT Module, you can model decay, but cannot model any reactants.

## Modeling Higher Order Reactions

GoldSim was designed to simulate first-order decay reactions. Note, however, that by defining the decay rate as a function of concentration(s), higher order reactions can also be represented.

For example, suppose you wanted to simulate the following reaction within GoldSim:



in which the reaction was second order:

$$d[A]/dt = -k [A]^2$$

where  $[A]$  is the mole concentration of A in the Cell of interest and  $k$  is the second order rate constant, with units of  $[(\text{mole}/\text{m}^3)^{-1} \text{yr}^{-1}]$ . First, of course, you would specify that B was a daughter of A. How then, would you represent the second order reaction rate?

In this case, we could rewrite the rate law as:

$$d[A]/dt = -\{k c_A / MW_A\} [A] = -k' [A]$$

where  $c_A$  is the *mass* concentration, and  $MW_A$  is the molecular weight.  $k'$  then represents a "pseudo first-order" rate constant. Specifying the "pseudo first-order" decay rate for A as the function " $(k) (MW_A)/A_A$ " has the effect of simulating the second-order rate law.

Note that defining the decay rate as a function of the concentration creates a recursive model (since the dissolved concentration is a function of the decay rate, and the decay rate is a function of the dissolved concentration). Hence, when you do this, you must utilize a previous value element. Previous value elements are discussed in detail in Chapter 10 of the **GoldSim User's Guide**. As discussed in that section, you must take extra care when simulating systems with previous value elements to ensure that your timestep is appropriately small.



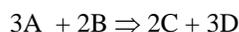
**Note:** In order to model reactants, you must have the RT Module. If you are using the CT Module, you can model decay, but cannot model any reactants.

## Representing Stoichiometry

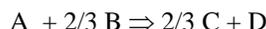
GoldSim specifically allows you to define stoichiometry for reactions.

**Read more:** [Defining Species Decay Properties](#) (page 52).

For example, suppose one wished to simulate the following reaction within GoldSim:



which can be written equivalently as



Assume here that the rate law is as follows:

$$d[A]/dt = -k [A]^3 [B]^2$$

In this case, we could rewrite the rate law with respect to A as:

$$d[A]/dt = -\{k (c_A/MW_A)^2 (c_B/MW_B)^2\} [A] = -k_A' [A]$$

Similarly, we could rewrite the rate law with respect to B as:

$$d[B]/dt = -\{(2/3) k (c_A/MW_A)^3 (c_B/MW_B)\} [B] = -k_B' [B]$$

where  $k_A'$  represents a pseudo first-order rate constant with respect to A, and  $k_B'$  represents a pseudo first-order rate constant with respect to B. This reaction would then be simulated within GoldSim as follows:

1. Specify the decay rate for A as the function  $k_A'$ ;
2. Define C and D as daughters of A, with a specified stoichiometric ratio of 2/3 for C and 1 for D; and
3. Specify the decay rate for B as the function  $k_B'$ , with no daughter products.



**Note:** In order to model reactants, you must have the RT Module. If you are using the CT Module, you can model decay, but cannot model any reactants.



**Note:** GoldSim only allows four daughter products to be specified. Hence, this limits the number of reaction products which can be simulated to (4)\*(the number of reactants).

## Complex Reaction Example: Monod Kinetics

To illustrate the manner in which GoldSim can be used to represent complex higher order reactions, let's consider a problem involving *Monod kinetics*. Monod kinetics has been applied in systems where a microorganism population increases because a contaminant present in the environment supports the microorganism's growth. This particular example file, Monod.gsm, can be found in the Contaminant Transport Examples folder in your GoldSim directory (accessed by selecting **File | Open Example...** from the main menu).



**Note:** Because this example includes reactants, it requires the RT Module. If you are using the CT Module, you will not be able to open the file.

Assume we have a Cell containing 1 m<sup>3</sup> of Water, with an initial concentration of contaminant (4.6 g/m<sup>3</sup>), and an initial concentration of microorganisms (1E10 cells/m<sup>3</sup>). Assume a cell has a mass of 1E-10 g. If the system follows Monod kinetics, the rate of change of the contaminant and the microorganisms with time can be described as follows:

$$\frac{d[\text{contam}]}{dt} = \frac{\mu_{\text{max}} \cdot (\text{Bugs}) \cdot [\text{contam}]}{Y\{K_m + [\text{contam}]\}}$$

and

$$\frac{\left\{ \frac{d(\text{Bugs})}{dt} \right\}}{\left\{ \frac{d[\text{contam}]}{dt} \right\}} = Y$$

where:

(Bugs)	= concentration of microorganisms (cells/L <sup>3</sup> );
[contam]	= concentration of contaminant (mol/L <sup>3</sup> );
$\mu_{\max}$	= maximal growth rate (1/T);
$K_m$	= Monod constant (mol/L <sup>3</sup> ); and
Y	= constant yield (cells/mol).

This would be represented in GoldSim as follows:

1. Define two species (Contaminant and Bugs);
2. Specify that the Contaminant has Bugs as a daughter product, with a stoichiometry equal to the yield, Y (2E14 cell/mole). Because stoichiometry factors are dimensionless, Y must be divided by Avogadro's number, resulting in a stoichiometry factor of 3.321E-10 mole/mole).
3. The rate of change of the contaminant can be rewritten in terms of mass concentrations as:

$$\frac{d[\text{contam}]}{dt} = \left[ \frac{\mu_{\max} \cdot c_{\text{Bugs}}}{Y \cdot M_{\text{Bugs}} \left\{ K_m + \frac{c_{\text{contam}}}{MW_{\text{contam}}} \right\}} \right] [\text{contam}] = k' [\text{contam}]$$

where:

$c_{\text{contam}}$	= the concentration of the contaminant (M/L <sup>3</sup> );
$c_{\text{Bugs}}$	= the concentration of the microorganisms (M/L <sup>3</sup> );
$M_{\text{bugs}}$	= the mass of a single microorganism (M/cell); and
$MW_{\text{contam}}$	= the molecular weight of the contaminant (M/mole).

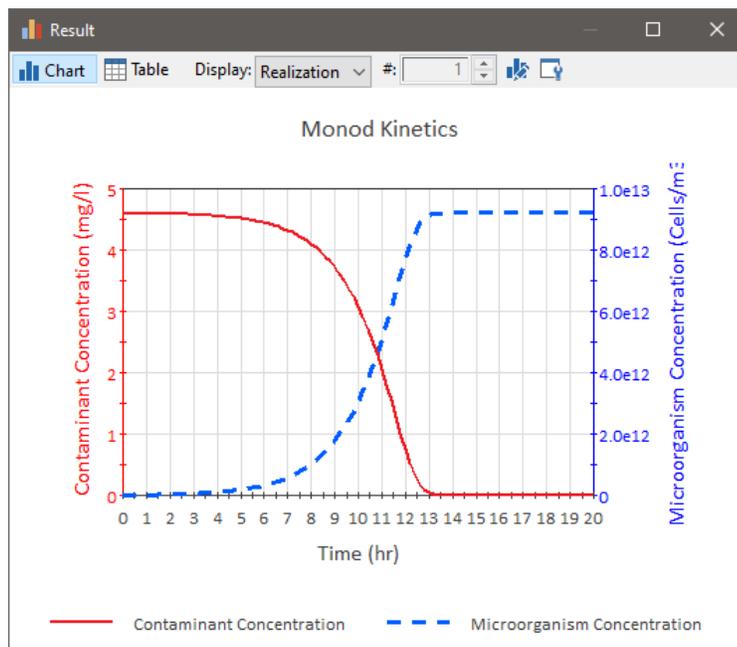
The  $k'$  term defined above can then be entered as the pseudo first-order decay rate for the contaminant. Assume  $\mu_{\max}$  is equal to 0.7 hr<sup>-1</sup>,  $K_m$  is equal to 6.4E-3 mole/m<sup>3</sup>, and the molecular weight of the contaminant is equal to 100 g/mol. Note that the "molecular weight" of the microorganisms is 1E-10 g/cell x Avogadro's number = 6.02E13 g/mol.

4. Define a single Cell containing 1 m<sup>3</sup> of Water;

5. Define an initial mass of contaminant in the Cell of 4.6 g, and an initial quantity of microorganisms of 1E10 cells. Assume the mass of one cell is equal to 1e-10 g.
6. Specify the simulation settings and run the model.

Note that defining the decay rate as a function of the concentrations creates a recursive model (since the concentration is a function of the decay rate, and the decay rate is a function of the concentration). Hence, when you do this, you must utilize a previous value element. Previous value elements are discussed in detail in Chapter 10 of the **GoldSim User's Guide**. As discussed in that section, you must take extra care when simulating systems with previous value elements to ensure that your timestep is appropriately small.

The output of this model, in the form of a time history of the contaminant and microorganism concentrations, is shown below:



## Competing Reactions

GoldSim can be used to simulate competing reactions. For example, suppose you wanted to simulate the following reaction:



where the forward rate of reaction was  $k_F$  and the reverse rate of reaction was  $k_R$ .

To simulate this, you would specify a decay rate of  $k_F$  for A with daughter product B, and a decay rate of  $k_R$  for B with daughter product A.

For this particular example, in a closed system at equilibrium, you would find that:

$$[A]/[B] = k_R/k_F$$

## Simulating Non-Chemical Constituents

Although the species in a GoldSim model will typically represent chemicals (man-made or naturally occurring), you can also use GoldSim to model the transport of other types of mass in an environmental system.

## Bacteria and Viruses

In most cases, you can treat microorganisms in the same way you would treat chemical species within GoldSim.

**Read more:** [Complex Reaction Example: Monod Kinetics](#) (page 301).

The key point to remember is that GoldSim always simulates species in terms of *mass*, whereas typically you will want to reference microorganisms in terms of the *number of cells* present. Hence, in order to simulate microorganisms, you will need to define the mass of a single cell, and enter all data in terms of the microorganism mass. You can subsequently use an element to convert results (e.g., concentrations) to be in terms of cells rather than mass

## Colloids and Particulates

In some cases, when attempting to simulate particulate or colloidal matter in GoldSim, it may be appropriate to simply treat them as another species.

In many cases, however, the colloids or particulates are actually more properly thought of as another medium. GoldSim has special features that allow you to represent particulates in Cells, Aquifers and Pipes.

**Read more:** [Defining Suspended Solids in a Cell](#) (page 124); [Simulating Suspended Solids in an Aquifer](#) (page 185); [Simulating Suspended Solids in a Pipe](#) (page 212).

In both cases, you define the particulate as a Solid medium (and hence the particulate can act as a storage and transport medium for species). You then directly specify a particulate mass (or for Pipes and Aquifers, a concentration) in each pathway.

Occasionally, you may want the particulates to act as a transport medium, but you may also wish to carry out a mass balance on the particulate concentration (i.e., you can't simply assume that it is constant). In order to do this, you could specify the particulate as a species *and* a medium. You would then define the concentration of the medium in a pathway by referencing the species concentration in the pathway. This would create a recursive system, and would necessarily involve the use of previous value elements (i.e., the medium concentration would be specified as the species concentration at the previous timestep). Previous value elements are discussed in Chapter 10 of the **GoldSim User's Guide**.

## Heat Transport

Heat transport is completely analogous to mass transport. Hence, *heat* can be simulated as a species in GoldSim. Note, however, that GoldSim treats all species in terms of *mass*. In order to simulate heat transport, therefore, you will need to enter data which reference heat (e.g., calories) as if it were mass (e.g., grams). The easiest way to do this is to assume, for the purpose of data entry and calculations, that 1 gram is equivalent to 1 calorie. At the end of your calculations, you can then multiply results by 1 cal/g so that they display in the proper units.

When simulating heat, the following points should be noted:

- The molecular diffusivity must be replaced by the *thermal diffusivity* (typically denoted as  $\kappa$ ). The thermal diffusivity is computed as follows:

$$\kappa = K/(\rho c_p)$$

where:

$\kappa$  = thermal diffusivity [m<sup>2</sup>/sec];

K = thermal conductivity [cal/(sec m °C)]

$\rho$  = density [kg/m<sup>3</sup>]; and

$c_p$  = specific heat [cal/(kg °C)].

- To convert computed “heat concentrations” in a fluid (in cal/m<sup>3</sup>) to temperature, it is necessary to divide the “heat concentration” by the product  $\rho c_p$ .
- To convert computed “heat concentrations” in a solid (in cal/kg) to temperature, it is necessary to divide the “heat concentration” by  $c_p$ .
- Partition coefficients between media for heat can be computed by assuming that at equilibrium, the temperature in all media is the same. The partition coefficient (which simply represents the ratio of concentrations) between solid A and fluid B is then:

$$K_{AB} = c_{p,A} / (c_{p,B} \rho_B)$$

where:

$K_{AB}$  = partition coefficient between solid A and fluid B [m<sup>3</sup>/kg];

$\rho_B$  = density of fluid B [kg/m<sup>3</sup>];

$c_{p,A}$  = specific heat of solid A [cal/(kg °C)]; and

$c_{p,B}$  = specific heat of fluid B [cal/(kg °C)].

Similarly, the partition coefficient between fluid C and fluid B is:

$$K_{CB} = (c_{p,C} \rho_C) / (c_{p,B} \rho_B)$$

where:

$K_{CB}$  = partition coefficient between fluid C and fluid B [m<sup>3</sup>/m<sup>3</sup>];

$\rho_C$  = density of fluid C [kg/m<sup>3</sup>]; and

$c_{p,C}$  = specific heat of fluid C [cal/(kg °C)].

- Note that the species heat could be produced by a reaction:



where n is the number of calories of heat produced per mole of A reacted.

If you also had to simulate heat conduction through a solid (e.g., conduction through the wall of pipeline), you could do so as follows:

- Give the solid (e.g., representing the pipeline material) an arbitrarily small fictitious porosity value.
- Define the tortuosity for the solid in such a way that it produces the correct heat flow (since in GoldSim, all of the transport is through the fluid phase):

$$\text{tortuosity} = \frac{\text{thermal conductivity of solid}}{\text{fictitious solid porosity} * \text{thermal conductivity of Fluid}}$$



---

# Appendix A: Introduction to Environmental Simulation

A little learning is a dangerous thing.

Alexander Pope, *An Essay on Criticism*

## Appendix Overview

This appendix provides a very brief introduction to environmental simulation. As used here, *environmental simulation* refers to modeling the transport and fate of various species (typically, but not necessarily, anthropogenic contaminants) through subsurface soils and rocks, surface waters, and the atmosphere.

This appendix makes no attempt to describe the physical and chemical processes controlling the fate and transport of such species, and in fact, assumes the reader already has some familiarity with these processes. Rather, the appendix describes an overall approach to carry out such simulations.

Because detailed discussion of this topic is well beyond the scope of this appendix, readers who are new to environmental simulation are strongly encouraged to consult additional literature. A number of excellent textbooks exist which focus on the overall approach to environmental simulation. Mackay (1991) provides a very good introduction. Schwarzenbach et al. (2003), while focusing on the detailed chemical and physical processes controlling the fate and transport of organic compounds, also includes an excellent chapter on environmental modeling.

### In this Appendix

This appendix includes discussions of the following topics:

- What is Environmental Simulation?
- Carrying out an Environmental Simulation: An Overview
- Developing a Conceptual Model
- Building the Mathematical Model
- Quantifying Input Parameters
- Documentation and Quality Assurance
- References

## What is Environmental Simulation?

The GoldSim Contaminant Transport Module is intended to facilitate simulations of environmental systems. As used here, the term “environmental system” can be defined as follows (Schwarzenbach et al., 1993):

*An environmental system is a subunit of the environment separated by a boundary from the rest of the world. The description of the system is comprised of the relations within the system as well as those characterizing the action of the outside world on the system.*

In an environmental simulation, we build an abstract representation or facsimile (i.e., a “simulation model”) of an environmental system in order to better understand those factors which control the system (e.g., contaminant properties such as solubilities or hydrogeological properties such as hydraulic conductivity) and/or to predict the future behavior of the system (e.g., the evolution of contaminant concentrations in a well).

By definition, any such system model is a simplification of reality, with the goals being to include those aspects that are assumed to be important and omit those which are considered to be nonessential, so as to derive useful predictions of system performance in an efficient manner.

If the environmental system includes some man-made component (such as a waste disposal facility), such an environmental simulation is often referred to as *performance assessment (PA)* or *safety assessment (SA)*, since one is attempting to predict the performance or the degree of safety of a particular facility. This terminology is most commonly used in conjunction with the evaluation of potential or existing hazardous or radioactive waste disposal facilities. For other environmental applications, such as predicting the fate of organic contaminants released to the environment, this is often referred to as *environmental transport modeling* or *multimedia environmental modeling*. Modeling the transport and fate of chemicals within an organism (e.g., humans) is referred to as *physiologically-based pharmacokinetic modeling (PBPK)*.

All of these kinds of environmental simulations can be readily represented using the GoldSim Contaminant Transport Module.

## Carrying Out an Environmental Simulation: An Overview

The specific steps involved in carrying out an environmental simulation are summarized below:

1. *Define your objectives and measures of performance.* Before attempting to simulate an environmental system, it is important to first clearly identify what types of questions you are trying to answer with the model. The objectives of the model define the performance measures for the system. A performance measure is a model output by which you can judge the performance of the system (e.g., the concentration of a particular contaminant at a specific location, a contaminant release rate from a specific source, or a dose to a particular receptor). Clearly identifying the objectives of the model will also help you determine the appropriate level of detail in the model.
2. *Develop the conceptual model.* The most important step in simulating any system is developing a conceptual model of the system. A conceptual model is a representation of the significant features, events

and processes controlling the behavior of the system. It is essentially a body of ideas, based on available information, that summarizes the current understanding of the system. Development of a conceptual model is typically the most time-consuming part of any environmental simulation effort.

**Read more:** [Developing a Conceptual Model](#) (page 310).

3. *Create the mathematical model.* Once a conceptual model of the system is developed, it is necessary to represent it quantitatively within a mathematical model. A mathematical model consists of a set of input assumptions, parameters, equations and algorithms describing the system.

**Read more:** [Building the Mathematical Model](#) (page 312).

4. *Quantify the input parameters.* The mathematical model identifies specific inputs (e.g., the flow rate in a river, or the financial discount rate) which are required in order to simulate the system. These must be quantified by specifying their values or probability distributions.

**Read more:** [Quantifying Input Parameters](#) (page 312).

5. *Implement and solve the mathematical model using a computational tool.* After developing the mathematical model and quantifying all of the input parameters, the model must be implemented within a computational tool capable of solving the equations representing the system. This implementation of the mathematical model within a computational tool is referred to as the simulation model. For simple systems, the computational tool might be your brain (if you can solve the equations in your head), a calculator, or perhaps a spreadsheet program. For more complex systems, a specialized computer program (such as GoldSim) is required.
6. *Document the model and evaluate, explain and present the results.* The final step in the simulation process is to produce results, evaluate and draw conclusions from these results, and document the model and present the results to interested parties.

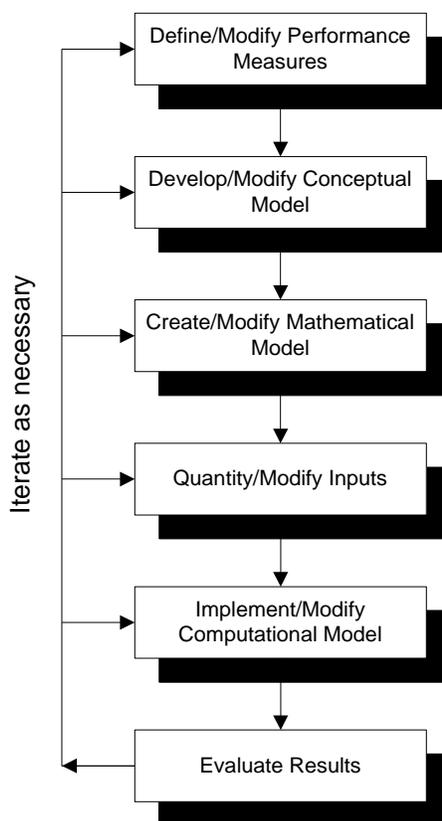


**Note:** Although expressed here in terms of environmental simulation, these steps are generally applicable to nearly any kind of simulation effort.

---

## Iterative Environmental Simulation

For very simple environmental simulations, the steps described above could be carried out in order, proceeding from step 1 to step 6. For most “real-world” simulations, however, these steps should be carried out in an iterative manner, responding to new information and/or model results. Such an iterative approach to environmental simulation is illustrated schematically below:



The basic concept is that as new data are obtained (e.g., from an environmental sampling program) and/or as new insights to the behavior of the system are obtained (based on preliminary model results), you should refine the model and reevaluate the system.

Environmental simulation models which are constructed and continuously modified in this manner can then do more than only provide predictions of performance; they can provide a systematic framework for organizing and evaluating the available information about the system, and can act as a management tool to aid decision-making with regard to data collection and resource allocation (what should be studied, when, and in what detail?).

## Developing a Conceptual Model

Because development of the conceptual model of a system is perhaps the most important step of any environmental simulation effort, it is worthwhile to discuss this step in somewhat greater detail.

As pointed out above, before attempting to simulate a system, it is important to clearly define the ultimate purpose and objective(s) of the model. The objectives of a model determine the measures by which the performance of the system will be evaluated. They also determine the amount of detail incorporated into the model, and where most of the effort in developing the model should be focused.

Note that the environmental system itself is only a subunit of the global environment, and it is therefore necessary to determine the physical limits and boundaries of the model. The system may be influenced by things outside of the system limits (i.e., boundary conditions), but does not model any impacts on

### Specifying Modeling Objectives and Defining the System

things outside of the system limits. As described by Schwarzenbach et al. (2003):

*An environmental system is a subunit of the world defined by the system boundary separating the system (“in”) from the rest of the world (“out”). The model describes the system as it responds to external influences (“forces”) but neglects the influence of the system on the outside world.*

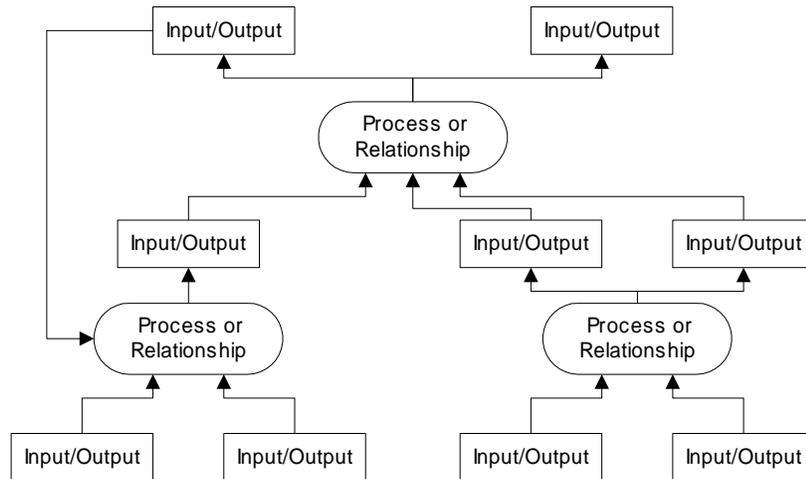
Hence, clearly defining the boundary between “in” and “out” is a critical first step in developing a conceptual model of a system.

## Describing Features, Processes and Events

Once the objectives of the model and the limits of the system are defined, an appropriate conceptual model for the system can be developed. As pointed out above, a conceptual model is a representation of the features, processes and events controlling the behavior of the system.

Conceptual model development for complex systems often centers on the creation of *influence diagrams*. Influence diagrams are graphical tools which provide a framework upon which a quantitative description of an environmental system can be constructed. The influence diagrams themselves can take many formats, depending on the personal preference of the individuals who develop and use them. Regardless of their format, their purpose is to present in a graphical manner the features, processes and events which may influence the system. They should be as comprehensive and robust as possible (incorporating items that may eventually be shown to have negligible contributions).

The following figure illustrates one way of developing influence diagrams:



This particular structure consists of two types of items: *processes or relationships* (represented by ovals), and *inputs/outputs* (represented by quadrilaterals). Inputs/outputs are intended to represent actual parameters, values or features (e.g., solubilities, volumes, lengths). Processes and relationships require input (e.g., hydraulic conductivity) and produce output (e.g., fluid flow rates). Hence, processes and relationships can be thought of as an equation (or group of equations) which acts to convert a set of input parameters into one or more output parameters. Outputs from one process or relationship may be inputs for another. In general, information flows upward in the influence diagram from lower level processes to upper level processes. As illustrated in the figure, however, it is possible for higher level processes to provide input for lower level processes (representing a feedback or coupling within the system).



**Note:** GoldSim’s graphical interface allows you, if you wish, to structure your models in the form of such an influence diagram.

---

The final step in constructing an influence diagram is to assess the significance of each component. Components which can be shown to have little significance can then be “pruned” from the model. Sometimes components may be pruned because their consequences or influence are minor; sometimes (for events) they may be pruned because they have a very low likelihood of occurring.

Influence diagrams typically form part of the documentation for a conceptual model. Often, however, the *process* of creating the influence diagrams is more useful than the end product itself. This is because the act of constructing an influence diagram forces the modeler or modeling team at the outset of the project to step back and look at the “big picture” and view the entire integrated system with all of its interconnections and couplings, as opposed to focusing on specific system details.

## Building the Mathematical Model

Once the conceptual model is developed and documented, it must be incorporated into a mathematical framework. The end product of incorporating a conceptual model into a mathematical framework is referred to here as a *mathematical model*. A mathematical model consists of a set of input assumptions, parameters, equations and algorithms for describing the system. In general, there should be a one to one correspondence between the conceptual model and the mathematical model. That is, every feature, process and event considered to be significant in the conceptual model should be quantitatively represented in the mathematical model.

The mathematical model essentially represents the input for the computational tool. It provides all the details necessary to simulate the system. As such, the mathematical model must typically be tailored to the specific computational tool in which it will be implemented. That is, the mathematical model is developed to take advantage of the assumptions, algorithms and features which are available in the computational tool.

Note that the mathematical model for a system will often include *abstractions* from more detailed process level models. For example, one might run a detailed chemical equilibrium model in order to develop a response surface describing the solubility of a particular contaminant as a function of various system parameters (e.g., pH, redox conditions). Running detailed process level models to develop the abstractions may make up a significant portion of the conceptual and mathematical model development process.

## Quantifying Input Parameters

The mathematical model identifies specific inputs which are required in order to simulate the system. For an environmental simulation, these include such items as the geometry of the system, contaminant source inventories, hydrologic and/or hydrogeologic properties, and the physical and chemical properties of the environmental media and the contaminant species.

These must be quantified by specifying their values (or probability distributions). Significant effort must be put into clearly documenting and defending the values or distributions assigned to these input parameters. This is particularly the case for modeling studies carried out within a confrontational

environment (e.g., simulations that are carried out to evaluate the safety of a proposed disposal facility).

As discussed in Chapter 9 of the **GoldSim User's Guide**, GoldSim provides a number of features to assist you in documenting the inputs to your model.

When defining input parameters, it is important to quantify uncertainty and clearly differentiate ignorance regarding the value of a parameter from its inherent variability (in space or time). These issues are discussed in general terms in Appendix A of the **GoldSim User's Guide** ("Introduction to Probabilistic Simulation"). IAEA (1989) and Cullen and Frey (1999) provide detailed discussions on explicitly dealing with variability and uncertainty in environmental models.

*Read more:* [Representing Spatial Variability](#) (page 294).

## Documentation and Quality Assurance

Two aspects of environmental simulation that are sometimes inadequately addressed are documentation and quality assurance. Although each of these can be time-consuming, they are an essential aspect of carrying out a defensible environmental simulation, and should be explicitly addressed in planning documents and budgets associated with major environmental simulation efforts. They are discussed briefly below.

Proper documentation of an environmental simulation typically will include, in some form, four aspects:

- *A description of the environmental system*, reviewing what is known about it and the issues to be addressed by the model.
- *A description of the conceptual model*. Note that development and documentation of a conceptual model should be independent of the computational tool which is used to represent it. That is, the reader should not require knowledge of the computational tool which was used to represent the model.
- *A description of the mathematical model and definition and quantification of its input parameters*. This forms the key portion of the documentation, and should be thorough enough to allow the simulation to be independently reproduced. Note that although the description of a conceptual model is independent of the computational tool in which it is to be implemented, the description of a mathematical model typically is not. This is because the manner in which an equation is solved or a parameter is defined is often dependent on the specific assumptions and algorithms incorporated into the computational tool. As a result, the written description of a mathematical model typically assumes that the reader is familiar with the basic functions of the computational tool in which it is implemented. For example, if a mathematical model was implemented in a spreadsheet, the written description of the mathematical model typically would assume that the reader understands that data can be represented in columns and rows, and that specific functions (such as MIN, MAX or SUM) are incorporated in the computational tool.
- *A description of the results and implications of the simulation*. Like the conceptual model description, the discussion and presentation of the

### Documenting an Environmental Simulation

results can often be done in a manner that it is largely independent of the computational tool which was used.

The importance of adequate documentation cannot be overemphasized. This is particularly the case in the environmental field, where simulations are often used in conjunction with controversial projects (e.g., siting a waste disposal facility, determining liability, evaluating safety). A well documented environmental simulation should be transparent and easily understood by a reader who is technically competent, but not an expert in environmental simulation. In addition, the key portions of the documentation (e.g., summary of the conceptual model, conclusions and implications) should be easily understood by most non-technical readers (e.g., managers, decision-makers, concerned citizens).

### Quality Assurance Procedures

Quality assurance is a critical part of environmental simulation, particularly for large, complex applications. All such applications of a program such as GoldSim should be carried out under some type of quality assurance program. The details of a particular program will differ, depending on the user and the application, but should include, in some form, the following key aspects:

- *Independent technical review of the conceptual model.*
- *Independent technical review of the mathematical model.* This review should include verification that all significant aspects of the conceptual model are represented within the mathematical model.
- *Verification of the simulation model.* This consists of verifying that the mathematical model has been accurately input into the computational tool.
- *Technical review and verification of results.* This includes verifying that model results have been accurately reproduced in any presentation of the results (i.e., no errors have been made in transferring results from the simulation model to the document describing the results).
- *Documentation and back-up of input/output files.* All computer input and output files associated with the simulation model should be documented and saved to ensure that the model can be readily re-run and results can be reproduced at a later date.

## References

The references cited in this appendix are listed below:

Cullen, A.C. and H. C. Frey, 1999, Probabilistic Techniques in Exposure Assessment, Plenum Press, New York.

IAEA, 1989, Evaluating the Reliability of Predictions Made Using Environmental Transfer Models, IAEA Safety Series No. 100, International Atomic Energy Agency, Vienna.

Mackay, D., 1991, Multimedia Environmental Models: The Fugacity Approach, Lewis Publishers, Inc., Chelsea, Michigan.

Schwarzenbach, R.P., P.M. Gschwend and D.M. Imboden, 2003, Environmental Organic Chemistry, 2<sup>nd</sup> Edition, John Wiley & Sons, New York.

---

# Appendix B: Details of Pathway Computations

Do not worry about your difficulties in mathematics. I can assure you that mine are greater.

Albert Einstein

## Appendix Overview

This appendix presents the theoretical basis and the mathematical details of the transport pathways in GoldSim. Because the key assumptions upon which the behavior of transport pathways is based are presented in the main text (Chapter 4), an understanding of these details is not necessary in order to use the Contaminant Transport Module. Nevertheless, many experienced modelers will want to have a more detailed understanding of the governing equations and solution algorithms upon which the transport pathways are based, and that information is presented in this appendix.

### In this Appendix

This appendix includes discussions of the following topics:

- Cell Pathway Details
- Pipe Pathway Details
- Plume Function Details
- Aquifer Pathway Details
- Network Pathway Details
- References

## Cell Pathway Details

The governing equations for Cell pathways and the manner in which these equations are solved by GoldSim are discussed below.

### Mass Balance Equation for Cell Pathways

The basic mass balance equation for Cell *i* is as follows:

$$m'_{is} = -m_{is}\lambda_s + \sum_{p=1}^{NP_s} m_{ip}\lambda_p f_{ps} R_{sp} \left( \frac{A_s}{A_p} \right) + \sum_{c=1}^{NF_i} f_{cs} + S_{is} \quad (\text{B-1})$$

where:

$m'_{is}$	=	rate of increase of mass of species <i>s</i> in Cell <i>i</i> [M/T];
$m_{is}$	=	mass of species <i>s</i> in Cell <i>i</i> [M];
$\lambda_s$	=	decay rate for species <i>s</i> [T <sup>-1</sup> ];
$NP_s$	=	number of direct parents for species <i>s</i> ;
$f_{ps}$	=	fraction of parent <i>p</i> which decays into species <i>s</i> ;
$R_{sp}$	=	stoichiometric ratio of moles of species <i>s</i> produced per mole of species <i>p</i> decayed;
$A_s$	=	molecular (or atomic) weight of species <i>s</i> [M/mol];
$A_p$	=	molecular (or atomic) weight of species <i>p</i> [M/mol];
$NF_i$	=	number of mass flux links from/to Cell <i>i</i> ;
$f_{cs}$	=	influx rate of species <i>s</i> (into cell <i>i</i> ) through mass flux link <i>c</i> [M/T]; and
$S_{is}$	=	rate of direct input of species <i>s</i> to Cell <i>i</i> from “external” sources [M/T].

The first term on the right-hand side in Equation (B-1) represents decay (or chemical reaction); the second term represents ingrowth; the third term represents mass transfer in or out of the Cell via mass flux links; and the fourth term represents the rate of direct input to the Cell from other sources.

The system of equations described in Equation (B-1) is coupled in two ways: 1) through the ingrowth terms, which couple all species in a decay chain; and 2) through the mass flux terms, which couple all Cells that are connected by mass flux links.

The rate of input from “external” sources ( $S_{is}$ ) includes things such as inputs directly specified by the user (i.e., the user can directly specify an initial condition, a fixed concentration and/or a mass flux rate into each Cell). For the purpose of the present discussion, these should be thought of as “uncoupled” inputs to the Cell (i.e., these inputs are not influenced by the computed concentration in the Cell).

A particular advective or diffusive mass transfer connection *c* is defined by a pair of pathways, a medium in each pathway, and a flux type:

medium **m** in pathway **i** ⇔ **flux type** ⇔ medium **n** in pathway **j**

The flux type can be advective or diffusive. Representation of the mass flux terms ( $f_{cs}$ ) is the most complex part of Equation (B-1), and is described in detail below.

## Advective Mass Flux Links

For an advective mass flux link from Cell  $i$  to Cell  $j$ , the flux of species  $s$ ,  $f_s$ , is computed as follows:

$$f_{s,i \rightarrow j} = c_{ims} q + \sum_{t=1}^{NPT_{im}} PF_t \cdot c_{its} \cdot vm_t \cdot cp_{imt} q \quad (B-2)$$

where:

- $q$  = the rate of advection (of the medium) for the mass flux link  $L^3/T$  for fluid mass flux links and  $M/T$  for solid mass flux links];
- $c_{ims}$  = the total dissolved, sorbed or precipitated concentration of species  $s$  in medium  $m$  within Cell  $i$  [ $M/L^3$  if  $m$  is a fluid;  $M/M$  if  $m$  is a solid];
- $NPT_{im}$  = the number of solid media suspended in medium  $m$  within Cell  $i$ ;
- $PF_t$  = Boolean flag (0 or 1) which indicates whether advection of solid  $t$  suspended in the advecting fluid  $m$  is allowed for the mass flux link;
- $c_{its}$  = the sorbed concentration of species  $s$  in solid medium  $t$  within Cell  $i$  [ $M/M$ ];
- $vm_t$  = the advective velocity multiplier for solid particulate  $t$
- $cp_{imt}$  = the concentration of suspended solid particulate  $t$  within fluid  $m$  in Cell  $i$  [ $M/L^3$ ];

The user directly specifies the medium flow rate when the flux link is defined in GoldSim. Note that by definition,  $q$  cannot be a negative number (i.e., an advective mass flux link can only flow one way). When you specify that a solid is present in a Cell as suspended particulate matter, it is assumed to be suspended in the first fluid that precedes it in the list of media for the Cell. Hence, the concentration of the solid particulate within the preceding fluid can be directly computed by GoldSim based on the masses and volumes of the media which are present.

**Read more:** [Defining Suspended Solids in a Cell](#) (page 124).

The second term (the summation) in Equation (B-2) accounts for the advection of suspended solids in a fluid. Note that for solid advective connections, the second term is not applicable (i.e.,  $PF_t = 0$ ).

Transport of particulates within an advecting fluid *from* a Cell *to* a receiving pathway is allowed ( $PF_t = 1$ ) if:

- the receiving pathway is not a Cell; or
- the receiving pathway is a Cell and the solid exists in the receiving pathway (although it need not be suspended in a fluid in the pathway).

If the solid does not exist in the receiving pathway, the second term is set to zero and conceptually, the particulates are effectively “filtered” out of the flux link and not transported out of the Cell.

The manner in which the concentrations (e.g.,  $c_{ims}$ ,  $c_{its}$ ) are computed for each species in each medium in a Cell is discussed below.

**Read more:** [Computing Concentrations in Cells](#) (page 323).

## Direct-Transfer Mass Flux Links

Direct transfer mass flux links simply transfer a specified fraction, per unit time, of the contents of one Cell to another. They are similar to advective links,

except that instead of specifying the flow rate for a fluid or solid medium, you specify a vector (on the species set) of fractional transfer rates, with dimensions of 1/time.

For a direct transfer mass flux link from Cell i to Cell j, the flux of species s,  $f_{s,i \rightarrow j}$ , is computed as follows:

$$f_{s,i \rightarrow j} = T_{ij,s} m_{is} \quad (\text{B-3a})$$

where:

$T_{ij,s}$  = the ‘turnover rate’ for species s, which represents the fraction of s in Cell I that is transported to Cell j per unit time [ $T^{-1}$ ];

$m_{is}$  = the total mass of species s in Cell i [M]

### **Precipitate Removal Mass Flux Links**

Precipitate-transfer mass flux links transfer a specified fraction, per unit time, of the precipitated mass in one Cell to another. They are similar to advective links, except that instead of specifying the flow rate for a fluid or solid medium, you specify a fractional transfer rate, with dimensions of 1/time.

For a precipitate transfer mass flux link from Cell i to Cell j, the flux of species s,  $f_{s,i \rightarrow j}$ , is computed as follows:

$$f_{s,i \rightarrow j} = T_{ij} m_{is}^p \quad (\text{B-3b})$$

where:

$T_{ij}$  = the ‘turnover rate’ for precipitates, which represents the fraction of precipitated masses in Cell i that is transported to Cell j per unit time [ $T^{-1}$ ];

$m_{is}^p$  = the precipitated mass of species s in Cell i [M]

### **Treatment Mass Flux Links**

Fraction-of-inflows (treatment) mass flux links intercept and transfer a specified fraction, per unit time, of the external inputs into one Cell to another Cell. They are similar to advective links, except that instead of specifying the flow rate for a fluid or solid medium, you specify a vector (on the species set) of interception efficiencies. “External inputs” refers to the following:

- Influxes coming from non-Cell elements such as Pipes, Pipe-networks, and External Pathways.
- Influxes coming from ‘normal’ or ‘previous value’ type links from other Cell elements. Specifying one of these link types forces the originating Cells to be in different Cell-nets from the receiving Cell.

Note that coupled influx links from other Cells are NOT included in the intercepted amounts.

For a fraction-of-inflows mass flux link from Cell i to Cell j, the flux of species s,  $f_{s,i \rightarrow j}$ , is computed as follows:

$$f_{s,i \rightarrow j} = T_{ij,s} m'_{is} \quad (\text{B-3c})$$

where:

$T_{ij,s}$  = the ‘treatment efficiency’ for species s, which represents the fraction of incoming mass of species s entering Cell i that is transported to Cell j;

$m'_{is}$  = the external inflow rate of species s into Cell i [ $MT^{-1}$ ]

## Diffusive Mass Flux Links

Diffusive mass flux links are used to transport mass through a stagnant or slowly moving fluid via the process of molecular diffusion. Diffusive mass transport is driven by (in fact, proportional to) a concentration difference, with mass diffusing from high concentration to low concentration. The constant of proportionality is referred to as the *diffusive conductance*:

$$\text{Diffusive Mass Rate} = (\text{Diffusive Conductance}) * (\text{Concentration Difference})$$

In this equation, the Diffusive Mass Rate has dimensions of mass/time, the Diffusive Conductance has dimensions of volume/time, and the Concentration Difference has dimensions of mass/volume.

The diffusive conductance is a function of the properties of the species and fluids involved (multiple fluids can be involved), and the geometry of the diffusive process.

Assuming that the species are diffusing through a single fluid, the Diffusive Conductance term is computed as follows:

$$D = (A d t n r) / L$$

where:

A is the mean cross-sectional area of the connection ( $L^2$ );  
 D is the Diffusive Conductance ( $L^3/T$ );  
 d is the diffusivity in the fluid ( $L^2/T$ );  
 n is the porosity of the porous medium;  
 t is the tortuosity of the porous medium;  
 r is a reduction factor, that varies with saturation (1 if saturated);  
 L is the diffusive length (L).

d and r are Fluid properties, and t and n are Solid properties.

The diffusive flux  $f_{s,i \rightarrow j}$  from pathway i to pathway j is computed as follows:

$$f_{s,i \rightarrow j} = D_s \left( c_{ims} - \frac{c_{jns}}{K_{nms}} \right) + \sum_{t=1}^{NPT_{im}} PF_t \cdot D_t (c_{its} \cdot cp_{int} - c_{jts} \cdot cp_{jnt}) \quad (B-4)$$

where:

$D_s$  = diffusive conductance for species s in the mass flux link [ $L^3/T$ ];  
 $c_{ims}$  = the dissolved concentration of species s in medium m within Cell i [ $M/L^3$ ];  
 $c_{jns}$  = the dissolved concentration of species s in medium n within Cell j [ $M/L^3$ ];  
 $K_{nms}$  = partition coefficient between fluid medium n (in Cell j) and fluid medium m (in Cell i) for species s [ $L^3$  medium m /  $L^3$  medium n];  
 $NPT_{im}$  = the number of particulate solid media in fluid m within Cell i;  
 $PF_t$  = Boolean flag (0 or 1) which indicates whether diffusion of solid t suspended in the fluid is allowed for the mass flux link;  
 $D_t$  = diffusive conductance for particulate t in the mass flux link [ $L^3/T$ ];

- $C_{its}$  = the sorbed concentration of species  $s$  associated with solid  $t$  within Cell  $i$  [M/M];
- $cp_{imt}$  = the concentration of solid particulate  $t$  within fluid  $m$  in Cell  $i$  [M/L<sup>3</sup>];
- $c_{jts}$  = the sorbed concentration of species  $s$  associated with solid  $t$  within Cell  $j$  [M/M]; and
- $cp_{jnt}$  = the concentration of solid particulate  $t$  within fluid  $n$  in Cell  $j$  [M/L<sup>3</sup>].

The first term in Equation (B-4) accounts for diffusion of dissolved species, while the second term accounts for diffusion of particulates suspended in the fluid. Note that diffusion can occur in either direction, so the flux can be positive or negative.

When you specify that a solid is present in a Cell as suspended particular matter, it is assumed to be suspended in the first fluid that precedes it in the list of media for the Cell. Hence, the concentration of the solid particulate within the preceding fluid can be directly computed based on the masses and volumes of the media which are present.

**Read more:** [Defining Suspended Solids in a Cell](#) (page 124).

The fluid media involved in Cells  $i$  (medium  $m$ ) and  $j$  (medium  $n$ ) need not be identical (i.e., intermedia diffusion is allowed). The  $K_{nms}$  term in Equation (B-4) allows for such intermedia diffusion, and is computed as follows:

$$K_{nms} = \frac{K_{nrs}}{K_{mrs}} \tag{B-5}$$

where:

- $K_{mrs}$  = partition coefficient between fluid medium  $m$  and reference fluid  $r$  for species  $s$  [L<sup>3</sup> fluid  $r$ /L<sup>3</sup> fluid  $m$ ]; and
- $K_{nrs}$  = partition coefficient between fluid medium  $n$  and reference fluid  $r$  for species  $s$  [L<sup>3</sup> fluid  $r$ /L<sup>3</sup> fluid  $n$ ].

Note that if  $K_{nms}$  is equal to zero (i.e., the species will not partition between the specified media), the diffusive flux is set equal to zero.

The diffusive conductance terms are computed as follows:

$$D_s = \frac{A}{\frac{L_i}{f_{ms} \cdot d_{ms} \cdot t_{Pi} \cdot r_m(\theta_m) \cdot n_{Pi}} + \frac{L_j}{f_{ns} \cdot d_{ns} \cdot t_{Pj} \cdot r_n(\theta_n) \cdot n_{Pj} \cdot K_{nms}}} \tag{B-6}$$

where:

- $A$  = the area of the diffusive mass flux link [L<sup>2</sup>];
- $L_i$  = diffusive length for the diffusive mass flux link in Cell  $i$  [L];
- $L_j$  = diffusive length for the diffusive mass flux link in Cell  $j$  [L];
- $f_{ms}$  = available porosity for species  $s$  in medium  $m$  ( $\leq 1$ );
- $f_{ns}$  = available porosity for species  $s$  in medium  $n$  ( $\leq 1$ );

$d_{ms}$	=	diffusivity for species s for fluid m (in Cell i) [ $L^2/T$ ];
$d_{ns}$	=	diffusivity for species s for fluid n (in Cell j) [ $L^2/T$ ];
$t_{pi}$	=	tortuosity for the porous medium defined for the diffusive mass flux link in Cell i ( $\leq 1$ );
$t_{pj}$	=	tortuosity for the porous medium defined for the diffusive mass flux link in Cell j ( $\leq 1$ );
$r_m(\theta_m)$	=	diffusive reduction formula for fluid m (in Cell i) to account for saturation level;
$r_n(\theta_n)$	=	diffusive reduction formula for fluid n (in Cell j) to account for saturation level;
$\theta_m$	=	Saturation of fluid m (in Cell i);
$\theta_n$	=	Saturation of fluid n (in Cell j);
$n_{pi}$	=	porosity for the porous medium defined for the diffusive mass flux link in Cell i;
$n_{pj}$	=	porosity for the porous medium defined for the diffusive mass flux link in Cell j; and
$K_{nms}$	=	partition coefficient between fluid medium n (in Cell j) and fluid medium m (in Cell i) for species s [ $L^3$ medium m / $L^3$ medium n].

GoldSim internally computes the saturation of the fluid in each Cell ( $\theta_m$  and  $\theta_n$ ), and uses this value to compute the diffusive reduction formula. The manner in which the diffusive reduction formula varies with saturation is specified directly by the user. Conceptually, the Diffusive Reduction Formula should equal 1 when the saturation is equal to 1 (and 0 when the saturation is equal to 0).

For each Cell, the saturation level of each fluid is computed by GoldSim as follows:

1. The combined pore volume of all (non-suspended) Solid media is computed as:

$$\text{Combined Pore Volume} = \Sigma (\text{Mass of Solid} * \text{Porosity} / \text{Bulk Density})$$

where the summation is over all solids.

2. For the first Fluid in the Cell, the Saturation is computed as:

$$\text{Saturation} = \min(\text{Fluid Volume}, \text{Combined Pore Volume}) / \text{Combined Pore Volume}$$

3. If there are additional fluids in the Cell, the Saturation for each Fluid is computed, in turn, as:

$$\text{Saturation} = \min(\text{Fluid Volume}, \text{Remaining Unfilled Pore Volume}) / \text{Combined Pore Volume}$$

This method of computing saturation has two important implications:

- The first Fluid listed in the Cell is treated as the wetting fluid (it is the first fluid to fill the pores).
- If the Cell contains multiple Solids, the fluids have access to the pore space in all the Solids simultaneously (i.e., the pore spaces of Solids are not filled in a specific order).



**Note:** The impact of saturation on the diffusion rate is complex. While the Diffusivity Reduction Formula reduces the effective diffusivity, a lower saturation changes the volume of water available. This in turn affects the concentration (and hence the concentration gradient). Moreover, decreasing the volume of water available increases the retardation due to sorption (since all of the mass of the porous medium is still assumed to be available, but only a fraction of the water is).

For suspended particulates, the diffusive conductance term is computed as follows:

$$D_t = \frac{A}{\frac{L_i}{d_{mt} \cdot t_{Pi} \cdot r_m(\theta_m) \cdot n_{Pi}} + \frac{L_j}{d_{nt} \cdot t_{Pj} \cdot r_n(\theta_n) \cdot n_{Pj}}} \quad (\text{B-7})$$

where  $A$ ,  $L_i$ ,  $L_j$ ,  $t_{Pi}$ ,  $t_{Pj}$ ,  $r_m(\theta_m)$ ,  $r_n(\theta_n)$ ,  $n_{Pi}$ , and  $n_{Pj}$  are as defined previously, and

$d_{mt}$  = diffusivity for particulate  $t$  within fluid  $m$  (in Cell  $i$ ) [ $L^2/T$ ];

$d_{nt}$  = diffusivity for particulate  $t$  within the fluid  $n$  (in Cell  $j$ ) [ $L^2/T$ ];

Equation (B-7) does not contain a partitioning term because, as will be discussed below, intermedia diffusive transport is not allowed for suspended particulates.

Diffusion of particulates *from* a Cell *to* a receiving pathway is allowed ( $PF_{ct} = 1$ ) if:

- the receiving pathway is not a Cell; or
- the receiving pathway is a Cell and the same fluid exists on both sides of the link and the solid exists in the receiving pathway (although it need not be suspended in a fluid in the pathway).

Hence, if the solid does not exist in the receiving pathway, or if the diffusive mass flux link involves two different fluids (inter-media diffusion), the particulates are effectively “filtered” out of the flux link and not transported out of the Cell.

The manner in which the concentrations (e.g.,  $c_{ims}$ ,  $c_{its}$ ) are computed for each species in each medium in a Cell is discussed below.

**Read more:** [Computing Concentrations in Cells](#) (page 323).

### Uncoupled Diffusive Mass Flux Links

In general, GoldSim solves the equations for pathways that are connected by diffusive mass flux links simultaneously (i.e., treating them as a single coupled system of equations), since the flux depends on the concentration on both sides of the link. Cells joined by coupled links for a single cell net and are solved as a coupled system of equations.

**Read more:** [Solution Algorithm for a Cell Net](#) (page 327).

There is one instance, however, in which pathways connected by a diffusive mass flux link are not solved simultaneously (i.e., they are uncoupled):

- If a Cell is connected diffusively to a non-Cell pathway, then the concentrations in the non-Cell pathway ( $c_{jns}$  and  $cp_{jnt}$ ), as well as the

diffusive length ( $L_j$ ) are assumed to be zero. (Setting  $L_j$  to zero implies that there is no diffusive resistance on that side of the mass flux link.)

## Computing Concentrations in Cells

### Concentrations with No Solubility Constraints

When species mass enters a Cell, it is instantaneously partitioned among the media present in the Cell. The partitioning is controlled by the partition coefficients defined for each species in each medium, and the quantity of each medium present.

*In the absence of solubility limits*, the concentration of species  $s$  in Medium  $m$  in Cell  $i$  is computed by GoldSim as follows:

$$c_{ims} = \left( \frac{K_{mrs}}{\sum_{g=1}^{NM_i} K_{grs} \cdot VM_{ig}} \right) m_{is} \quad (B-8)$$

where:

- $c_{ims}$  = concentration of species  $s$  in medium  $m$  in Cell  $i$  [(M/L<sup>3</sup>) for Fluids or (M/M) for Solids];
- $m_{is}$  = mass of species  $s$  in Cell  $i$  [M];
- $K_{mrs}$  = partition coefficient between medium  $m$  and Reference Fluid  $r$  for species  $s$  [(L<sup>3</sup>/L<sup>3</sup>) for Fluids or (L<sup>3</sup>/M) for Solids];
- $K_{grs}$  = partition coefficient between medium  $g$  and Reference Fluid  $r$  for species  $s$  [(L<sup>3</sup>/L<sup>3</sup>) for Fluids or (L<sup>3</sup>/M) for Solids];
- $VM_{ig}$  = quantity (volume or mass) of medium  $g$  in Cell  $i$  [L<sup>3</sup> for Fluids or M for Solids]; and
- $NM_i$  = the number of media in Cell  $i$ .

Note that, by definition, for all species, the partition coefficient between the Reference Fluid and itself is 1 (i.e., in the above equation, if  $m$  is the Reference Fluid,  $K_{mrs} = 1$ ).

### Concentrations with Solubility Constraints

When a solubility constraint is applied for a species in a Cell, the Cell has a *saturation capacity* with respect to that species, which represents the maximum amount of species mass the Cell can contain before the species will start to precipitate out of solution.

The saturation capacity of a Cell is a function of the solubility limit in the reference fluid, the partition coefficients for the other media present in the cell, and the quantities of the media present in the cell:

$$msat_{is} = sol_{sr} \sum_{g=1}^{NM_i} K_{grs} \cdot VM_{ig} \quad (B-9)$$

where:

- $msat_{is}$  = saturation capacity for species  $s$  in Cell  $i$  [M];
- $sol_{sr}$  = solubility of species  $s$  in the Reference Fluid  $r$  [M/L<sup>3</sup>];
- $K_{grs}$  = partition coefficient between medium  $g$  and Reference Fluid  $r$  for species  $s$  [(L<sup>3</sup>/L<sup>3</sup>) for Fluids or (L<sup>3</sup>/M) for Solids];

$VM_{ig}$  = quantity (volume or mass) of medium  $g$  in Cell  $i$  [ $L^3$  for Fluids or  $M$  for Solids]; and

$NM_i$  = the number of media in Cell  $i$ .

If the total species mass in the Cell does not exceed the saturation capacity, the solubility limit has not been reached, and concentrations in the various media in the Cell are computed based on partition coefficients and media quantities as described in the previous section. If, however, the saturation capacity is exceeded, media concentrations are computed differently.

In particular, the element's concentration in the Reference Fluid is set to the solubility limit, and the concentrations in other media are computed based on their partition coefficients and the concentration in the Reference Fluid using Equation (B-8). In addition, the concentrations in Solids in the Cell are incremented by the amount of "precipitated" species mass (the difference between the total mass in the Cell and the saturation capacity).

Mathematically, this can be restated more precisely as follows:

- The concentration in the Reference Fluid is set to the solubility limit for species  $s$ ,  $sol_{sr}$  [ $M/L^3$ ];
- The dissolved concentration [ $M/L^3$ ] in all other Fluids in the Cell is computed as:

$$c_{ims} = sol_{sr} K_{mrs} \quad (B-10)$$

where  $K_{mrs}$  is the partition coefficient between fluid  $m$  and Reference Fluid  $r$  for species  $s$  [dimensionless].

- The concentration [ $M/M$ ] in *suspended (particulate)* Solids ( $c_{its}$ ) is computed as:

$$c_{its} = sol_{sr} K_{trs} \quad (B-11)$$

where  $K_{trs}$  is the partition coefficient between solid  $t$  and Reference Fluid  $r$  for species  $s$  [ $L^3/M$ ].

- The concentration [ $M/M$ ] in Solids *which are not suspended* ( $c_{ims}$ , where  $m$  is a solid) is computed as:

$$c_{ims} = sol_{sr} K_{mrs} + \frac{(mtot_{is} - msat_{is})}{\sum_{h=1}^{NS_i} VM_{ih}} \quad (B-12)$$

where  $K_{mrs}$  is the partition coefficient between solid  $m$  and Reference Fluid  $r$  for species  $s$  [ $L^3/M$ ],  $mtot_{is}$  is the total mass of species  $s$  in Cell  $i$  [ $M$ ],  $msat_{is}$  is the saturation capacity of species  $s$  in Cell  $i$  [ $M$ ],  $VM_{ih}$  is the mass of (non-suspended) Solid  $h$  in Cell  $i$ , and  $NS_i$  is the number of non-suspended Solids in Cell  $i$ .

Note the difference between the treatment of suspended Solids and those that are not suspended. In particular, for computational reasons, the mass in the Cell in excess of the saturation capacity (the "precipitated" mass) is assumed to be precipitated only onto those Solids which are not suspended. Hence, although species mass can be partitioned onto (and transported with) particulate Solids, *precipitated* species mass is never associated with suspended Solids.

If you are simulating multiple isotopes of the same element, GoldSim must handle the solubility calculations in a special way. This is because, physically, solubility is actually an element property (as opposed to a species property).

**Read more:** [Entering Media Properties for Isotopes of the Same Element](#) (page 80).

Therefore, GoldSim does the following:

1. It assumes that the solubility entered for the first isotope of the element in the species list is the correct solubility. The solubility of each other isotope of the same element should be proportional to its atomic weight; if it is not in the correct ratio a warning message is generated.
2. It uses the sum of the (mole-normalized) masses of all isotopes of an element to determine if the element saturation capacity has been exceeded; and
3. If the element saturation capacity has been exceeded, it "shares" the element solubility in the Reference Fluid among the isotopes of the element based on the isotopic ratios. (For example, if the uranium isotopes  $^{235}\text{U}$  and  $^{238}\text{U}$  were present in a Cell at an isotopic ratio of 2 to 1, and the total mass of uranium in the Cell exceeded the saturation capacity, the dissolved concentration of  $^{235}\text{U}$  would be computed as 2/3 of the element uranium solubility.)

Note that as a result of these relationships, decay-chains that share isotopes of a common element become coupled if the element exceeds its solubility limit. We use the term 'decay-family' to refer to sets of decay chains that have elements in common. GoldSim automatically accounts for this coupling by solving the cell-net equations for entire families simultaneously. When a multi-isotope element reaches its solubility limit in a cell, GoldSim generates a linearized first-order solution of the fully-coupled equations for the family. This solution requires a bigger matrix, but is more accurate and allows longer substeps. The substeps are automatically limited by allowable maximum changes in isotope ratios.

**Read more:** [Solution Algorithm for a Cell Net](#) (page 327).

### Calculating Effective Concentrations in Fluids with Suspended Solids

If one or more Solids are suspended in a Fluid, GoldSim computes and displays an *effective concentration* for the fluid (as the Concentration\_in\_Fluid output for the Cell), which includes the contribution from suspended solids.

This effective concentration in the fluid is computed as follows:

$$ce_{ims} = c_{ims} + \sum_{t=1}^{NT_{im}} \frac{mp_{it}}{VM_{im}} c_{its} \quad (\text{B-13})$$

where:

- $ce_{ims}$  = the effective concentration of species  $s$  in fluid  $m$  in Cell  $i$  ( $\text{M}/\text{L}^3$ );
- $c_{ims}$  = the dissolved concentration of species  $s$  in fluid  $m$  in Cell  $i$  ( $\text{M}/\text{L}^3$ );
- $mp_{it}$  = the mass of suspended particulate solid  $t$  in Cell  $i$  ( $\text{M}$ );
- $VM_{im}$  = the volume of the fluid  $m$  in Cell  $i$  ( $\text{L}^3$ );
- $c_{its}$  = the concentration of species  $i$  in particulate solid  $t$  in Cell  $i$  ( $\text{M}/\text{M}$ ); and
- $NT_{im}$  = the number of solids suspended in fluid  $m$  in Cell  $i$ .

## Impact of Available Porosity on Cell Pathway Behavior

You can assign Available Porosities to Solids.

**Read more:** [Advanced Solid Properties](#) (page 77).

The Available Porosity is entered separately for each species, and represents the fraction of the pore volume of the Solid that is accessible to each species.

An Available Porosity less than 1 indicates that some of the volume is inaccessible for that species. Implementing an available porosity which is less than 1 may be appropriate when simulating Cell Pathways involving media such as clay, where processes such as anion exclusion may be active.

Specifying a fractional Available Porosity for a solid affects GoldSim in two ways:

1. The volume of fluid accessible to the species is reduced (the volume in the inaccessible pore space is ignored). In particular, the quantity of Reference Fluid in equations (B-8), (B-9), (B-12) and (B-13) is adjusted as follows:

$$VM_{irs} = VM_{ir} - \sum_{m=1}^{NS_i} \frac{(1 - f_{ms}) n_{im} VM_{im}}{\rho_{im}} \quad (B-14)$$

where:

- $VM_{irs}$  = the volume of reference fluid r in Cell i which is accessible to species s ( $L^3$ );
- $VM_{ir}$  = the actual volume of reference fluid r in Cell i ( $L^3$ );
- $VM_{im}$  = the mass of solid m in Cell i (M);
- $f_{ms}$  = the available porosity for species s in medium m;
- $n_{im}$  = the porosity of medium m in Cell i;
- $\rho_{im}$  = the dry density of medium m in Cell I ( $M/L^3$ ); and
- $NS_i$  = the number of solids in Cell i.

Changing the volume of fluid available affects the degree of partitioning between solids and fluids



**Warning:** GoldSim does not force consistency between the specified volume for the reference fluid and the specified porosity, density and mass of the solids. As a result, it is possible that you could inadvertently specify inputs such that the right hand side of Equation (B-14) was negative. Although GoldSim will prevent the effective volume from going negative (it sets it equal to zero), the result is unlikely to be what you intended. Hence, when using fractional available porosities it is critical that you define the quantities of media present in each Cell in a manner that is consistent with the properties of the solid representing the porous medium (i.e., density and porosity).

2. For diffusive mass fluxes in which the Solid is specified as the porous medium, the effective diffusivity for the element of interest on that side of the connection is multiplied (reduced) by the Accessible Porosity. This is indicated in Equation (B-6).



**Note:** The impact of specifying a fractional available porosity for a solid on mass transfer rates is complex. For diffusive mass flux links (and matrix diffusion zones) in which the Solid is specified as the porous medium, the effective diffusivity for the element of interest is multiplied (reduced) by the Accessible Porosity. However, the volume of fluid available to the species is reduced. This in turn affects the concentration (and hence the concentration gradient for diffusive mass flux links). Moreover, decreasing the volume of fluid available increases the retardation due to sorption (since all of the mass of the porous medium is still assumed to be available, but only a fraction of the fluid is).



**Note:** You cannot assign an available porosity to a particulate. Hence, when particulates diffuse into or out of a Cell, the full porosity of the porous medium is always available.

## Solution Algorithm for a Cell Net

In order to solve the coupled equations represented by Equation (B-1), GoldSim initially identifies the sub-networks of interconnected (coupled) Cells, referred to as *cell nets*, which then are treated as single entities in the calculations. A cell net is defined by all Cells that are interconnected via coupled mass flux links.

GoldSim sets up and solves a separate set of fully-coupled equations for each cell net. Hence, the fluxes between cells *within* a cell net are computed simultaneously (since they are solved as a system of coupled differential equations). Fluxes *between* cell nets (or between cell nets and non-Cell pathways), however, are uncoupled. At each timestep, GoldSim solves the upstream system, solves for its mass outfluxes, and then solves the downstream system.

Within a cell net, the equations for any species that are part of a decay chain are also coupled. Also, when solubility limits for multi-isotope elements are exceeded, their decay-chains become coupled. GoldSim sets up a separate set of coupled differential equations for each *decay family* in each cell net. (A decay family consists of all decay chains that have elements in common.) The resulting matrix differential equations (B-1) can be expressed for a single decay family in a cell net as follows:

$$\mathbf{m}' = [\mathbf{D} + \mathbf{T}]\mathbf{m} + \mathbf{S} \quad (\text{B-15})$$

where:

- m** = the vector of the masses of each species in the family in each Cell in the net [M];
- m'** = the vector of rates of increase of mass of each species in the family in each Cell in the net [M/T];
- D** = a matrix containing the decay and ingrowth coefficients [1/T];
- T** = a matrix containing the mass transfer coefficients (through mass flux links) [1/T]; and
- S** = a vector of the input rates from external sources of each species in the family in each Cell in the net [M/T], and correction terms for any species which have exceeded their saturation capacities.

Note that the “external sources” (**S**) include all mass inputs external to the cell net (i.e., from Source elements and pathways outside of the cell net).

Cell elements with specified concentrations do not have positions in the matrix equations. Their impact on the solution is incorporated in the **S** vector for external sources, using the transport terms for their mass flux links, Equations B-2 and B-4.

Applying the backwards-difference (fully implicit) algorithm for the timestep  $\Delta t$  results in:

$$\mathbf{m}(t + \Delta t) = [\mathbf{I} - \Delta t \mathbf{D} - \Delta t \mathbf{T}]^{-1} \{\mathbf{m}(t) + \Delta t \mathbf{S}(t)\} \quad (\text{B-16})$$

where **I** is the identity matrix. In the absence of solubility limits, these equations are linear and each decay chain’s equations are uncoupled.

GoldSim uses an iterative, sparse-matrix solver to solve equation B-16.

For a system with time-varying properties, the **T** matrix in Equation B-16 is constructed as follows:

- All mass flux parameters (except media flow rates) use the values at time  $t + \Delta t$  (i.e., the solution is fully implicit).
- Media flow rates use the values at time  $t$ . This is because these should be computed by Reservoirs or Pools which use an explicit solution scheme (i.e., they are forward looking rather than backward looking).
- When the amounts of the media are changing during a timestep, a constant *effective* value (representing a weighted average of the media amount at the beginning and end of the timestep) is used for the amount of each medium. (Note that this weighting is not applied to models run with Low Precision. For Low Precision, the volume at time  $t + \Delta t$  is used.)

**Read more:** [Solving the Matrix Equations Numerically](#) (page 331).

The equations GoldSim solves for each net are defined in terms of *nodes*, where a node represents either a Cell in the cell net (primary nodes) or monitored discharges from the net (secondary nodes). GoldSim defines a secondary node for any mass flux link for which it needs to compute the flux rate:

- mass flux links to non-Cell pathways or to other cell nets;
- mass flux links within a cell net for which the user has requested that results be saved; and
- mass flux links that are referenced in other elements (e.g., Sum or Extrema elements).

The secondary nodes simply act to “receive” transported species mass.

Partitioning Equation (B-16) according to primary and secondary nodes (with subscript 1 referring to primary nodes and subscript 2 referring to secondary nodes) results in the following, which is the basic equation which is solved for each decay family by GoldSim:

$$\begin{Bmatrix} \mathbf{m}_1(t + \Delta t) \\ \mathbf{m}_2(t + \Delta t) \end{Bmatrix} = \begin{bmatrix} \mathbf{I}_{11} - \Delta t \mathbf{D}_{11} - \Delta t \mathbf{T}_{11} & 0 \\ -\Delta t \mathbf{T}_{21} & \mathbf{I}_{22} \end{bmatrix}^{-1} \begin{Bmatrix} \mathbf{m}_1(t) + \Delta t \mathbf{S}_1(t) \\ 0 \end{Bmatrix} \quad (\text{B-17})$$

Note that the  $\mathbf{I}_{22}$  term implies that mass discharged from the cell-net stops being decayed at the instant it exits. The decay process is resumed in the next downstream pathway as the mass enters it. The discharged mass from an upstream pathway is assumed to be uniformly distributed over the length of the time step when it is applied to the downstream pathway.

The solution to (B-17) is:

$$\mathbf{m}_1(\mathbf{t} + \Delta\mathbf{t}) = [\mathbf{I}_{11} - \Delta\mathbf{t}\mathbf{D}_{11} - \Delta\mathbf{t}\mathbf{T}_{11}]^{-1} \{\mathbf{m}_1(\mathbf{t}) + \Delta\mathbf{t}\mathbf{s}_1(\mathbf{t})\} \quad (\text{B-18a})$$

and

$$\mathbf{m}_2(\mathbf{t} + \Delta\mathbf{t}) = -\mathbf{T}_{21}\mathbf{m}_1(\mathbf{t} + \Delta\mathbf{t}) + \mathbf{m}_2(\mathbf{t}) + \Delta\mathbf{t}\mathbf{s}_2(\mathbf{t}) \quad (\text{B-18b})$$

Note that the term  $\mathbf{m}_2(\mathbf{t})$  is zero at the start of each step. However, if fractional steps are used in the solution, this term is no longer zero following the first fractional step. GoldSim uses 4 fractional steps for its medium-precision option, and 10 fractional steps for its high-precision option.

In the absence of solubility constraints, the matrix equations (B-16) are linear. If, however, solubility constraints are being simulated, the equations for a cell net change (and become non-linear) when an element reaches its solubility limit in a Cell.

### **Solving the Matrix Equations with Solubility Constraints**

Where there are advective and/or diffusive flux links between two cells in a net, the net mass flux between the cells can be expressed as the sum of two one-way fluxes, which are functions of the mass of species in the cell at each end of the link. In general:

$$\mathbf{f}_{i \rightarrow j} = \mathbf{t}_{i \rightarrow j} \mathbf{m}_{s,i} + \mathbf{s}_i \quad (\text{B-19})$$

where:

- $\mathbf{f}_{i \rightarrow j}$  = (gross) flux of the species from cell i to cell j
- $\mathbf{t}_{i \rightarrow j}$  = transfer coefficient for movement of the species from cell i to cell j
- $\mathbf{m}_{s,i}$  = mass of the species in question in cell i
- $\mathbf{s}_i$  = constant term

Note that  $\mathbf{t}_{i \rightarrow j}$  is based on the  $\mathbf{f}_{cs}$  terms defined in equation (B-1) and detailed in (B-2) through (B-12). The  $\mathbf{t}_{i \rightarrow j}$  coefficient represents the combined effects of partitioning and advective, direct transfer and diffusive transport links. The term  $\mathbf{s}_i$  represents the sum of the  $\mathbf{s}_{is}$  terms from equation (B-1) plus various constant terms that appear in the flux equations when the species' element mass exceeds its concentration limit in cell i.

For purely advective or direct transfer transport from cell i to cell j, equation (B-19) represents the entire flux, whereas for diffusive transport there would be a corresponding flux in the reverse direction ( $\mathbf{f}_{j \rightarrow i}$ ), driven by the mass in cell j.

Internally, GoldSim calculates and saves arrays of transfer coefficients for each element and combination of cells in a net. Two sets of transfer coefficients are calculated: one set for fluxes of dissolved and/or sorbed species, and a second set of coefficients for the flux of species that are precipitated onto solids that may advect. These sets of transfer coefficients are then used when the mass-transfer matrix  $\mathbf{T}$  is assembled.

The mass-transfer matrix  $\mathbf{T}$  is assembled in the following way: for each cell in the net and species in turn, the coefficients controlling mass transfer of the species from that cell to each other linked cell in the net are calculated and

added to the matrix, along with the constant terms for the right-hand-side vector **S**. This is equivalent to adding the  $t_{i \rightarrow j}$  and  $s_j$  coefficients into the matrix and vector. Where there is a diffusive link between two cells, the reverse-direction coefficients (i.e. for flux from cell  $j$  to cell  $i$ ) are added when cell  $j$  is processed.

While the element mass in the cell  $i$  is below the solubility limit, equation (B-19) has the following form:

$$f_{i \rightarrow j} = t_{i \rightarrow j}^{ds} m_{s,i} \quad (\text{B-19a})$$

Where  $t^{ds}$  represents the dissolved and/or sorbed transport of the element.

When the solubility limit is exceeded, the equation is more complex:

$$f_{i \rightarrow j} = t_{i \rightarrow j}^{ds} \frac{m_{s,i}}{M_i} M_i^s + t_{i \rightarrow j}^p \left[ m_{s,i} - \frac{m_{s,i}}{M_i} M_i^s \right] \quad (\text{B-19b})$$

where:

- $M_i$  = total element mass in the cell, in moles
- $M_i^s$  = amount of the element that causes saturation, in moles
- $t_{i \rightarrow j}^p$  = is the transfer coefficient for transport of precipitated mass of the element

Unfortunately, equation (B-19b) is nonlinear, due to the  $m_{s,i} / M_i$  term, and thus it is significantly more difficult to solve than (B-19a). In the GoldSim's "family-by-family" algorithm, GoldSim's approach is to set up a linearized form of the equation, based on a first-order (McLaurin) expansion about a reference point. The initial reference point is defined as the cell isotopic masses when the solubility limit is first reached. Subsequently, while the element remains saturated, an updated reference point is used whenever the isotopic masses change significantly.

Collecting terms in equation (B-19b) and dropping the subscripts "i" and "i→j" for clarity, gives:

$$f = \left[ t^p + (t^{ds} - t^p) \frac{M^s}{M} \right] m_s \quad (\text{B-20})$$

For the first order expansion, the reference point is denoted by an overline. The expansion is:

$$f \cong t^p m_s + (t^{ds} - t^p) \frac{M^s}{M} \bar{m}_s + (t^{ds} - t^p) M^s \sum_{is} \left[ \frac{\partial}{\partial m_{is}} \left( \frac{m_s}{M} \right)_{ref} (m_{is} - \bar{m}_{is}) \right] \quad (\text{B-21})$$

where the derivative terms are evaluated at the reference point.

The summation term at the end of (B-21) can be expanded as:

$$\begin{aligned}
& \sum_{is} \left[ \frac{\partial}{\partial m_{is}} \left( \frac{m_s}{M} \right)_{\text{ref}} (m_{is} - \bar{m}_{is}) \right] \\
&= \frac{m_s - \bar{m}_s}{M} - \frac{\bar{m}_s}{M^2} \sum_{is} \frac{(m_{is} - \bar{m}_{is})}{w_{is}} \\
&= \frac{m_s - \bar{m}_s}{M} - \frac{\bar{m}_s}{M^2} \sum_{is} \frac{m_{is}}{w_{is}} + \frac{\bar{m}_s}{M}
\end{aligned} \tag{B-22}$$

where  $w_{is}$  is the molecular weight of species  $is$ .

Note that  $m_s$  is the mass of the species in question, while  $m_{is}$  refers to each isotope of the same element, inclusive of the species in question. Substituting the expanded summation term into (B-21) and simplifying gives:

$$\begin{aligned}
f \cong & \left[ t^p + (t^{ds} - t^p) \frac{M^s}{M} \right] m_s - \left[ (t^{ds} - t^p) \frac{M^s \bar{m}_s}{M^2} \sum_{is} \frac{m_{is}}{w_{is}} \right] \\
& + (t^{ds} - t^p) \frac{M^s}{M} \bar{m}_s
\end{aligned} \tag{B-23}$$

$$\text{or } f \cong \left[ t^p + \bar{C} \right] m_s - \frac{\bar{C} \bar{m}_s}{M} \sum_{is} \frac{m_{is}}{w_{is}} + \bar{C} \bar{m}_s \tag{B-24}$$

$$\text{where } \bar{C} = (t^{ds} - t^p) \frac{M^s}{M}$$

Equation (B-24) identifies the diagonal, off-diagonal, and constant terms in the matrix formulation used in GoldSim's family-by-family algorithm for isotopes of saturated elements.

### Solving the Matrix Equations Numerically

To solve the matrix equations, GoldSim uses a customized version of the Iterative Methods Library IML++, version 1.2a, available from the National Institute of Standards web site <http://math.nist.gov/iml++/>. This library provides a number of alternative sparse-matrix solution algorithms. While these algorithms are generally robust and efficient, on occasion an algorithm may become unstable or fail to converge. To minimize this possibility, GoldSim uses a two-stage solution approach. In the first stage, the Biconjugate Gradient Stabilized method is employed. If this fails for any reason, then a message is placed in the log file and the Generalized Minimum Residual algorithm is applied instead.

The backwards difference (fully implicit) algorithm has the advantages of being unconditionally stable, conserving mass, and having bounded error levels. In order to enhance the accuracy of the backwards difference method, GoldSim automatically divides every time step into a number of *fractional timesteps*, depending on the user's selected precision level (discussed below). These fractional timesteps are used only when computing cell nets, and are not applied to other GoldSim model elements outside of cell nets (such as volumes or flow

rates) These other variables stay constant over the full timestep and do not change during the fractional timesteps.

This subdivision is invisible externally, and is applied even when the step itself has been shortened in order to reach a solubility limit. As pointed out above, the backwards difference method is unconditionally stable and conserves mass, so the use of these fractional timesteps simply provides a more precise solution.

The equations for a cell net change (and become non-linear) when a species reaches its solubility limit in a Cell. GoldSim monitors concentrations in the Reference Fluid. If the concentration for a species reaches the solubility limit, GoldSim applies a boundary condition, holding the dissolved concentration in the Reference Fluid at the solubility limit, and switches to the solubility-limited (saturated) form for the matrix equations.

After switching to the solubility-limited (saturated) equations, GoldSim monitors the total mass of the element in the Cell. If this ever falls below the amount needed to reach the solubility limit, GoldSim switches the equations back to their standard form.

To carry out these processes with precision, GoldSim automatically uses a search algorithm to find the exact point in time where the governing equations change, and it dynamically changes the timestep to a value which can be much shorter than the user-specified timestep. These *substeps* (which are determined by the selected Solution Precision) can be as small as 1e-8 times the actual timestep length. Note that the substeps are used only when computing cell nets, and are not applied to elements outside of cell nets.

Using the search algorithm, GoldSim does the following:

1. It attempts to identify the exact point in time at which a species (or element) changes its saturation state to or from saturated. The search succeeds if the “overshoot” across the solubility limit is less than a specified fraction of the limit. If the overshoot exceeds this, the substep is reduced. This is repeated until the overshoot is less than the specified tolerance, or a minimum substep is reached. The overshoot tolerance and the minimum substep are determined by the Solution Precision.
2. It checks that the relative fractions of isotopes of a saturated element do not change excessively during a timestep. Similarly to changing the solubility state, GoldSim carries out a search in time trying to limit the change in isotopic fractions to a specified fraction of the value when the boundary conditions were last calculated. This fraction is determined by the Solution Precision. (This check is only carried out for isotopes present in the Cell in quantities greater than 1µg AND representing more than 1% of the total element mass).
3. It checks for a condition where an initially saturated species or element discharges mass at such a high rate that even at the shortest possible substep it calculates a negative remaining mass (of more than 1µg) in the cell at the end of the timestep. If the amount of mass in the Cell is negative at the end of the substep, GoldSim sets it to zero (*which has the effect of creating mass in the system*, as the “downstream” pathway will still retain the mass it received), and records a warning message in the Run Log.

Based on the solution precision setting (High, Medium or Low) defined in the Contaminant Transport tab of the **Model | Options** dialog, the solution parameters are set as follows:

Precision Setting	Low	Medium	High
Change in isotope ratios	.50	.30	.10
Solubility limit overshoot	.10	.05	.025
Shortest timestep fraction	1E-6	1E-7	1E-8
Fractional timesteps	1	4	10
Weight media amounts during fractional timesteps	No	Yes	yes
Solver tolerance	1E-6	1E-7	3E-9
Solver mass tolerance (g)	1E-17	1E-19	1E-22

The meanings of the different parameters are as follows:

- **Change in isotope ratios:** No isotope of a saturated element is allowed to change its fraction of the total element mass by more than this amount in a single step. If this limit is exceeded, the step is shortened and the linearized equations are reformed. The total amount of the saturated element's mass is also prevented from changing by more than this ratio.
- **Solubility limit overshoot:** Elements are not allowed to overshoot their solubility limit by more than this fractional amount. If this limit is exceeded, the step is shortened.
- **Shortest timestep fraction:** GoldSim attempts to identify the exact point in time at which a species (or element) changes its saturation state to or from saturated. The search succeeds if the "overshoot" across the solubility limit is less than the "Solubility limit overshoot". If the overshoot exceeds this, the substep is reduced. This is repeated until the overshoot is less than the specified tolerance, or the minimum substep ("Shortest timestep fraction" times the actual timestep) is reached.
- **Fractional Timesteps:** The number of computational timesteps that each full timestep is automatically subdivided into when computing cell nets.
- **Weight media amounts during fractional timesteps:** This determines whether a weighted average of the previous and current timestep is used to compute media amounts (e.g., volumes) for the purpose of computing mass transfer rates for fractional timesteps.
- **Solver convergence tolerance:** The maximum fractional root-mean-square error in the calculated solution mass.
- **Mass tolerance (g):** If the total mass of family species in the cell-net is less than the limit, do not bother to do decay or transport calculations for the family.

The isotope ratio test and solubility limit test are used to automatically constrain the timestep. The solution algorithm will reduce a timestep down to a minimum of "Shortest timestep fraction" times the actual timestep in order to try to meet the criteria. If this is not successful, a warning message will be placed in the log file.

An additional technique used to ensure the accuracy of solutions is that GoldSim requires a certain minimum number of solver iterations before a solution will be accepted, even if the accuracy requirements is met. This minimum number varies with the degree to which the accuracy criterion is exceeded. If the root-mean-square error is much less than the tolerance, a single iteration will be accepted. However, if the error is only slightly less than the tolerance, 8 iterations are required. The minimum acceptable number of iterations is established dynamically, using the following formula:

$$\text{min} = 8 e^{0.2\ln(\text{resid}/\text{tol})}$$

where:

min is the minimum number of solver iterations;

resid is the root mean square error, and

tol is the required solver accuracy.

This requirement for a minimum number of solver iterations helps to ensure that calculated mass flux rates are accurate. Because mass flux rates are usually a function of differences in masses (concentrations) between connected Cells, getting accurate flux rates requires a higher level of precision than simply getting accurate masses. While this higher precision could be achieved by simply reducing the allowable error in the solution, this would result in significantly increased run times. The approach taken in GoldSim, of requiring a minimum number of iterations, appears to provide highly accurate and efficient solutions.

As pointed out above, in order to enhance the accuracy of the backwards-difference (fully implicit) method, GoldSim automatically divides every timestep into a number of *fractional timesteps*, depending on the user's selected solution precision level (and these fractional timesteps are used only when computing cell nets, such that other variables stay constant during the fractional timesteps).

Using fractional timesteps is a very computationally efficient way to enhance the accuracy of the solution. All of the factors changed by the solution precision can affect the accuracy, but for many models (in particular, those that don't involve solubility limits or isotopes), the effective timestep for the Cell calculations (determined by the number of fractional timesteps) is typically the most important. Hence, to achieve the same accuracy using a 1 day timestep with Medium Precision (4 fractional timesteps) would require a 0.25 day timestep without fractional timesteps (Low Precision). But in this case, the Medium Precision run would be much faster (typically by a factor of 2, and potentially much more). This is because 1) only the cell nets are updated during these fractional timesteps; and 2) numerically the fractional timesteps are computed via matrix calculations in such a way that it takes less computational effort than simply shortening the actual timestep.

However, adding fractional timesteps in this way can have a cost. The easiest way to understand why this is the case is to recall that the mass transfer terms (for advective and diffusive mass flux links) discussed earlier include concentration terms. For example, the advective mass transfer rate out of a Cell for any particular outflow is equal to  $QC$ , where  $Q$  is the flow rate and  $C$  is the Cell concentration. The concentration, in turn, requires a media amount (or amounts). For example, in the absence of partitioning,  $C = M/V$ , where  $M$  is the mass in the Cell and  $V$  is the water volume. When we apply a finite difference approximation in time to represent these equations, these terms (e.g.,  $M$ ,  $V$ ) have to be represented at a particular time (the current timestep or the previous

timestep). In an implicit approach, the M (and by default V) terms used to represent the advective mass transfer rate are those at the current timestep (rather than the previous).

We are solving these equations for M in each Cell (and hence these are obviously changing). But other variables (e.g., media amounts such as V) could also be independently changing over time (e.g., the volume of reference fluid in the Cell could be increasing or decreasing). You would typically be computing such amounts separately using Reservoir or Pool elements.

When fractional timesteps are used (4 for Medium Precision; 10 for High Precision), GoldSim is updating the value for M at every fractional timestep. However, the value for the media amounts (e.g., V) are not updated every fractional timestep (we only have values for the current and previous full timestep). Moreover, the nature of the fractional timestepping algorithm is such that each fractional timestep within a full timestep must use the same value for the variables such as volume (we can't, for example, interpolate between the two timesteps). However, using the value of the volume, for example, at the end of the full timestep to compute concentrations during a fractional timestep is not appropriate for all of the fractional timesteps (only for the last one). To address this, an approximation is used to handle systems in which the amount of media in the Cells is changing over a timestep and fractional timesteps are being used. Under these circumstances, an *effective value* is used to represent the amount of each medium for the purpose of computing concentrations during the fractional timesteps. The effective value is a weighted average of the values at the current and previous timestep:

$$V_{\text{eff}} = 0.375 * V_t + 0.625 * V_{t + \Delta t}$$



**Note:** There is no theoretical foundation for this weighting function. It was developed empirically by running a number of numerical experiments.

---

The use of an effective amount reduces the error in the computed concentrations (and hence mass transfer rates) used in each fractional timestep, but does not eliminate it completely (i.e., it is better than using the value at the end of the timestep for all fractional timesteps, but it is still an approximation). The errors will be small as long as the amount of media does not change significantly over a full timestep. However, when the media amounts do change significantly over a timestep, computed concentrations in a Cell can show jumps or drops (i.e., positive or negative “spikes”). For example, when the volume is dropping, not enough mass is moved out, so the concentration artificially increases, and when the volume is rising, too much mass is moved out, so the concentration artificially decreases. These can result in inaccurate mass transfer rates and can therefore propagate downstream producing additional inaccurate behavior. Such errors are a consequence of the fractional timestepping algorithm and rapidly changing media amounts.



**Note:** The weighting function is only used for Medium and High Precision. For Low Precision, the amount is not weighted (the value at the current timestep is used). As a result running a model with Low Precision will not produce concentration jumps or spikes as Cell media amounts change (although, as discussed below, it does not eliminate mass errors and artificial spikes that can occur when a Cell completely empties, and also may require a smaller timestep).



**Note:** GoldSim monitors the fractional change in the volume (resulting from outflows) every timestep for the Reference Fluid and writes a warning message if this is too high (>10%). For most systems, the volume change will likely need to be higher than this to produce a significant error, but the warning is conservatively displayed at 10%. Note that the warning message is not repeated (it is only shown when it first exceeds 10%). Hence, the fractional change may actually be much greater than 10%.



**Note:** The warning message is only written for the Reference Fluid. If a different medium changes by more than 10% over a timestep due to outflows, no warning is written. Note also that this warning is not displayed when using Low Precision (for reasons described in the next section).

---

These errors are most significant when the amount of media in a Cell is low and rapidly changing (e.g., in which case the fractional change is by definition high).

If a Cell completely empties (the media amount goes to zero), an additional problem arises. In particular, when a Cell empties, some mass will be left in the Cell after it has emptied (on the order of the amount of mass present in the media at the last timestep just before the Cell emptied).



**Note:** Of course, if the Cell emptied at least partially due to evaporation (which would not be unusual, for example, for a surface water body that went dry), some mass realistically would in fact be left behind in the Cell, since evaporation does not transport mass (and mass would eventually precipitate out of solution as water evaporated). The discussion above, however, refers to the fact that even if the Cell empties due to outflows that transport mass (and there is no evaporation), mass will be (unrealistically) left behind for numerical reasons.

---

This issue of leaving mass behind in an empty Cell occurs whether or not fractional timesteps are used (i.e., it also occurs in the absence of fractional timesteps when Low Precision is specified).

The problem arises because, as pointed out above, the implicit solution method uses the media amount at the end of the timestep (or, in the case of Medium and High Precision, a weighted amount) to compute the mass transfer rate at the time the Cell goes empty. As a result, during the timestep at which the Cell goes empty, the mass transfer rate is either zero (for Low Precision, since we cannot compute a concentration if the media amount is equal to zero) or is too low (for Medium and High Precision, since we have used a weighted media amount that overestimates the media amount and therefore underestimates the concentration

and hence the rate). Hence, during that final timestep before the Cell empties we either transfer no mass out at all (Low Precision) or too little mass (Medium or High Precision). That is, in all cases, some mass is left in the Cell (Low Precision leaving more mass than Medium Precision, and Medium more mass than High Precision).

Even if only a very small amount of mass is left behind in the Cell, the problem can be compounded after the Cell goes empty in that any mass that may continue to enter the Cell would be unable to leave (for example, if the Cell was empty, but inflow was equal to outflow), since it is not possible to compute a concentration in a media when the amount of media is zero, and hence it is not possible to compute a mass transfer rate. If the Cell then refills, any mass left behind in the Cell (or collected in the Cell after it emptied) would be released suddenly (and this could result in unrealistic mass transfer rates and concentration spikes).



**Note:** GoldSim writes a warning message if the amount of media in a Cell goes to zero. If the amount of media in a Cell goes to zero and that media is involved in a diffusive mass flux link, a fatal error occurs (the model will not run).

---

**The manner in which these errors associated with rapidly changing (and, in the extreme, emptying) Cell media amounts can be minimized is discussed in the next section.**

---



**Note:** To keep this in perspective, it should be noted that in the real-world, the behavior of solutes in a system in which a Cell was emptying would likely be extremely complex, and hence very difficult (if not impossible) to model accurately. This is because the processes controlling concentrations as a Cell empties are often difficult to accurately represent. In particular, in most cases, one of the key outflows for a Cell that is emptying (e.g., a pond) would be evaporation. In such a case, solutes would indeed precipitate out of solution before the Cell emptied (and therefore be left behind in the Cell). Moreover, during this period (and the period when the Cell was refilling), the geochemistry of this high concentration solution would be quite complex indeed.

---

In general, with the exception of the discussion above related to rapidly changing media amounts within a timestep (or emptying Cells), users can rely on the algorithms described above to compute accurate results. As a result, the user does not generally need to be concerned with the length of the full timesteps that are used by GoldSim (since accuracy in the mass transport calculations can be improved by increasing the solution precision), provided that they are sufficient to adequately describe any changing boundary conditions (and media amounts).

There is one exception to this, and that is where the user requires a precise calculation of a small remaining fraction of a decayed species. In such a case the user may need to specify an increased number of timesteps in order to get precise results.

The reason for this is that GoldSim's solution manages the errors in the calculated changes in species masses from one time step to the next, rather than the error in the absolute value of the resulting masses. For a rapidly decaying species that went through 20 half-lives, a mass of 1 kg would decay to 0.954e-7

**Minimizing Errors for Systems with Rapidly Changing Media Amounts**

kg, so that the change in mass was -0.999 999 046 kg. Even if GoldSim accurately estimated the change in the mass to five significant figures, for example as -0.999 99, it would predict a new mass of  $1e-5$  kg— over ten times the exact value. In one sense this solution would be very accurate, but in another sense it would be very inaccurate. Users faced with problems like this, where they need to accurately compute the residual values of decayed species, should compare results obtained using successively increasing numbers of timesteps until the results have converged sufficiently.

As an example of this, a test was made where a species decayed through 20 half-lives, reducing its mass by a factor of  $2^{20}$ . Using high precision and just one GoldSim timestep, the resulting computed mass was 17.5 times larger than the exact solution. Using ten steps the result was 2.4 times too large, using 100 steps it was 1.1 times too large, using 1,000 steps its was 1.009 times too large, and using 10,000 steps it was 1.001 times too large.

In the previous section, we noted that rapidly changing Cell media amounts can result in errors in computed concentrations (and mass transfer rates).

These errors are most common and significant when the amount of media in a Cell is low and rapidly changing (in which case the fractional volume change is by definition high). If a Cell completely empties (the media amount goes to zero), an addition problem occurs. In particular, when a Cell empties, some mass will be left in the Cell after it has emptied (on the order of the amount of mass present in the media at the last timestep just before the Cell emptied). Moreover, if the Cell is empty by still has an inflow (with a matching outflow), mass will accumulate in the Cell. If the Cell then refills, any mass left behind (or accumulated) in the Cell would be released suddenly (and this itself could result in unrealistic spikes).

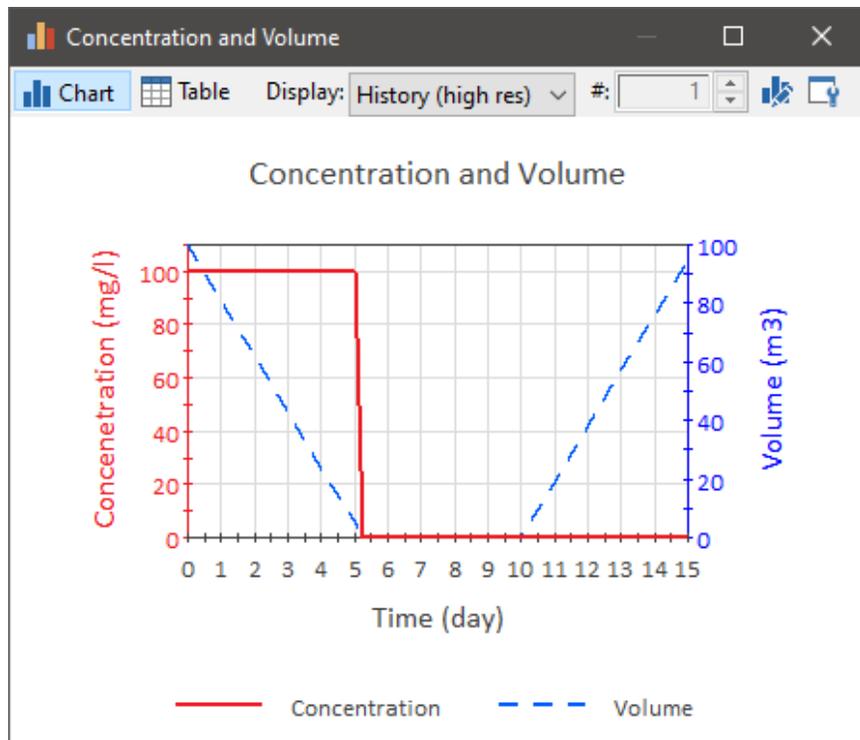
Fortunately, it is possible to minimize these errors by making some simple changes to the model. To illustrate this, it is easiest to consider a very simple example.



**Note:** These errors can manifest themselves in a variety of ways, and the magnitude of the errors can change depending on the system characteristics. This simple example, however, illustrates the key concepts involved and the approach described to minimizing the errors is completely applicable to more complex models.

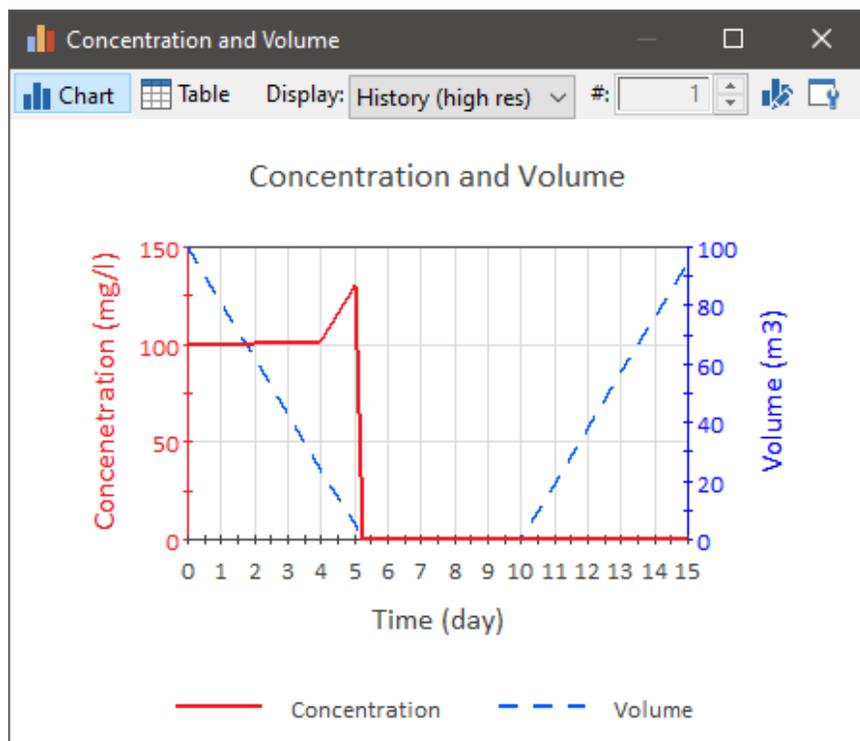
---

In this model, a pond starts with  $100 \text{ m}^3$  of water, and a concentration of 100 mg/l. No further mass is added. It has an outflow of  $19 \text{ m}^3/\text{day}$ , such that it empties a little after 5 days. At 10 days, an inflow of  $38 \text{ m}^3/\text{day}$  begins, along with an outflow of  $19 \text{ m}^3/\text{day}$  (such that there is a net outflow of  $19 \text{ m}^3/\text{day}$ ). The model is run with a 1 day timestep (but we will plot unscheduled updates, for example, inserted when the volume goes to zero). Conceptually, the system behavior should look like this:



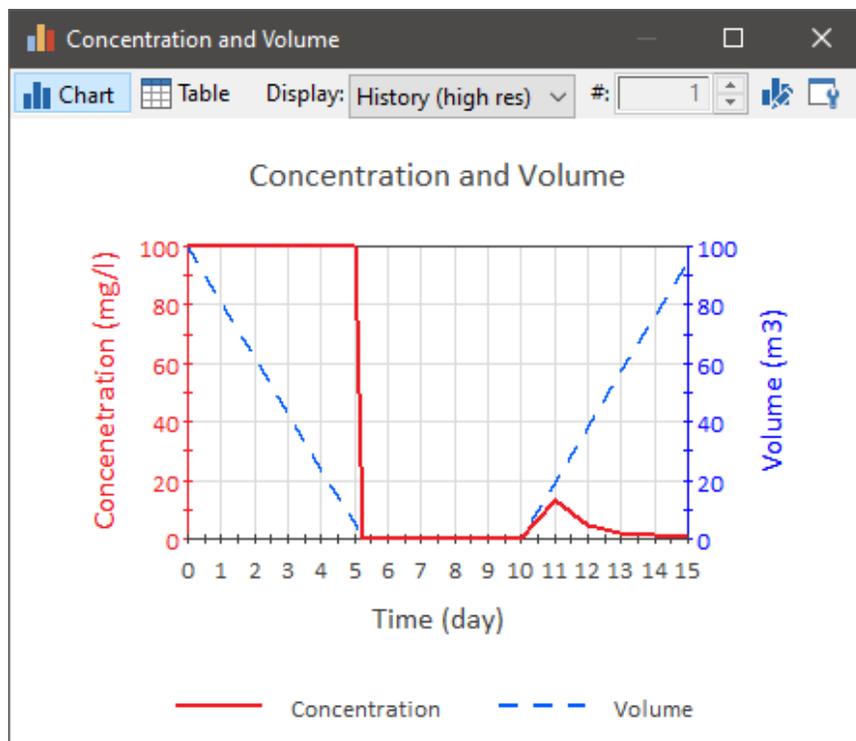
The concentration stays constant (we are not adding any mass and are removing water at the same rate as mass) until the Cell empties. When it empties, the concentration is actually undefined (there is no mass or volume), so it makes sense to report it as zero.

If we actually run the model with Medium Precision, the results look like this:



We see a spike just before the Cell empties (since too little mass is transferred out of the Cell as the fractional volume changes rapidly). A small amount of mass is also left in the Cell (not noticeable in this plot).

If we run the model with Low Precision (in which there are no fractional timesteps), the results look like this:

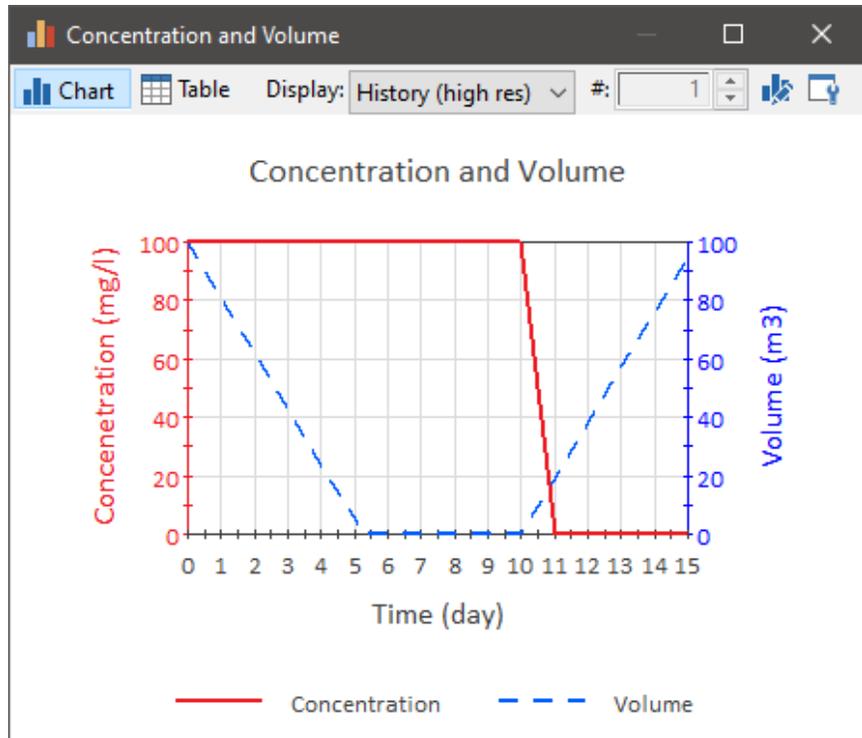


Here we see that there is no spike as the Cell empties, but we get a spike when the Cell starts to refill. This is because when the Cell emptied, although we were able to compute the concentration properly, mass was left behind in the Cell. When the Cell started to refill, this mass was suddenly flushed out. The Medium Precision case also has the same problem, but it always leaves a smaller amount of mass in the Cell when it empties, and in this particular example, the amount was small enough not to be noticeable.)

Our first step to address these errors is to prevent the media amount from going to zero. This can be done by defining a Lower Bound that is greater than zero for the Reservoir or Pool element representing the Cell media amount. When you do so, there will still be some mass left in the Cell (since some water will remain), but this can be minimized by defining an appropriately small value for the Lower Bound.

In this example, setting a Lower Bound of  $0.1 \text{ m}^3$  and running with Medium (or High) Precision actually makes the problem worse (the positive spike becomes quite high). As we shall see below, we need to make an additional change to address the problem.

However, simply setting a Lower Bound for Low Precision essentially eliminates the problem for this particular model:



What we see here is that the concentration (correctly) stays at 100 mg/l (since there is in fact now a small amount of mass and water in the Cell after it reaches the Lower Bound). The smaller the Lower Bound, the lower the amount of mass left behind. If you wanted to report zero concentration when the Cell was “empty” (at the Lower Bound), you could adjust the concentration when reporting it:

If(Volume = Lower Bound, 0 mg/l, Concentration)

Note that in this example, the mass in the Cell does go to zero when there is an inflow of clean water and an outflow at 10 days (and all mass is flushed). There is actually a very small concentration spike when the Cell starts to refill, but it is insignificant.

So based on this, you may think that the solution is simply to set a Lower Bound for the media amount and run the model with Low Precision. For some models, that would indeed be an appropriate solution. However, as pointed out in the previous section, the fractional timesteps provide an increase in accuracy in a very computationally efficient way.

And the solution precision can indeed have a significant impact. As a very simple illustration of this, consider a model in which we are computing the decay of 100 g of species with a half-life of 5 days in a Cell (with no inflows or outflows) for a period of 10 days, using a 1 day timestep. The solution is shown below:

Type	Value at 10 days (g)	% error
Analytical	25	-
Low Precision	27.3	9.2%
Medium Precision	25.6	2.4%
High Precision	25.2	0.8%

As can be seen, there is a significant accuracy improvement as the Precision Setting increases. In this simple example, to achieve the same accuracy as the Medium Precision run, a Low Precision run would require 4 times more timesteps. But the key point is that the Medium Precision run is not as computationally intensive as a Low Precision run with 4 times the number timesteps (required to achieve the same accuracy). How much less computationally intensive? It depends on the nature of the model (e.g., how many other elements not associated with the Cell network exist in the model), but the advantage is likely to be at least 2 and could in some cases be close to 4.

It is also important to understand that while in this simple decay example, the solution accuracy was only controlled by the number of fractional timesteps (1, 4 or 10), other variables controlled by the Solution Precision can play a role in more complex models (e.g., with different types of mass transport processes, more complex transient behavior, isotopes, solubility constraints, etc.).

The major point to keep in mind is that Medium and High Precision options add significant accuracy improvements in the solution of the mass transport equations with minimal computational expense. Hence, Low Precision runs, while effective at avoiding spikes, can have a cost in terms of accuracy. **For some models (particularly those with no solubility constraints, no rapidly decaying species and no isotopes) you could simply add a Lower Bound and run at Low Precision to avoid spikes. However, you may then need to decrease the size of the timestep to accurately solve the mass transport equations (and this would likely be more computationally intensive than using Medium Precision and dynamic adjustment of the timestep discussed above). Certainly for complex mass transport models (e.g., with rapidly decaying species, solubility constraints and/or isotopes), however, using Low Precision is not recommended.**

Therefore, what we would like to do is take advantage of the accuracy improvement of the Medium and High Precision setting (when Cell media amounts are not changing rapidly) while also avoiding the inaccurate behavior (when they are changing rapidly). That is, fractional timesteps used in Medium and High Precision simulations are a double-edged sword: they improve accuracy under most conditions, but produce spiky concentrations under some conditions (i.e., rapidly changing media amounts).

The approach to addressing this is to reduce the error to an acceptable level by dynamically adjusting the timestep only when these problems occur. **That is, we want to dynamically adjust (shorten) the timestep when the media amounts are changing significantly over a timestep due to advective outflows.**



**Note:** Although this error theoretically could impact both advective mass transfer (outflows) and diffusive mass transfer (as both require concentrations to be computed to compute the mass transfer rate), since the error requires relatively large fractional changes in media, practically, such changes will involve advection. Hence, our solution will focus on monitoring media changes and advective outflows in order to make sure we dynamically adjust the timestep to minimize errors. Moreover, it should also be noted that if the amount of any media (typically the Reference Fluid) that is involved in a diffusive mass flux goes to zero, a fatal error is issued (hence, you cannot create a Cell with diffusive connections whose media amount goes to zero).



**Note:** In most cases, the media amount we will be concerned with, of course, is the volume of the Reference Fluid (almost always water). Hence, in the discussion below, for simplicity, we will refer to the volume (of water), but the discussion applies to any media that is changing (and is involved in advective outflows).

As pointed out above, our goal is to dynamically adjust the timestep only when these problems occur. In particular, when we adjust the timestep, conceptually, we want to ensure that the following holds true:

$$\text{Rate of Volume Change} * \text{Timestep} < \text{Allowed Fraction} * \text{Current Volume}$$

The Allowed Fraction is the maximum allowable fractional change that we select to appropriately minimize the error. GoldSim provides a warning message if the fractional change is greater than 10%. However, for many systems, the fractional change will likely need to be higher than this to produce a significant error, but the warning is conservatively displayed at 10%. Experimentation will be required to determine the appropriate value. You want to use the largest value that minimizes the error to an acceptable level.

This defines the maximum timestep that we will allow as follows:

$$\text{Maximum Allowable Timestep} = (\text{Allowed Fraction} * \text{Current Volume}) / \text{Rate of Volume Change}$$

When should we apply this Maximum Allowable Timestep? First, we obviously need the Rate of Volume Change to be nonzero (to avoid a divide by zero error). However, we also want to have one other condition met: we want the total outflow over the next timestep to be a significant fraction of the current volume. This is because unless the outflow is significant, the error will not be significant (the error arises from the outflow term). We don't want to reduce the timestep, for example, if the volume was increasing due to inflows (and there were no outflows).

Hence, for any given timestep, we want to define a Maximum Allowable Timestep if 1) the volume is changing; and 2) the outflow over the next timestep would be a significant fraction of the current volume. That is, we want to shorten the timestep if these conditions are true:

$$\text{Rate of Volume Change (over the next timestep)} > \text{Zero}$$

AND

$$\text{Total Outflow over the next timestep} > \text{Allowed Fraction} * \text{Current Volume}$$



**Note:** These conditions will be true and most likely to shorten the timestep when: 1) the media amount is decreasing and approaching a (small) Lower Bound; and 2) there is an outflow but the media amount is increasing and leaving a small Lower Bound. They can also be true if there is a large outflow (that may or may not be matched by a large inflow) in which the volume is not close to the Lower Bound. As will be discussed below, however, this will not necessarily result in the timestep being shortened (even though the two conditions are met).

If both of these are true (and only if they are both true), we want to adjust the timestep to ensure that the rate of volume change over the timestep is sufficiently small.

Combining these conditions and this definition for the maximum step, we conceptually want to define the Maximum Allowable Timestep as follows:

```

If
    Volume change over next timestep > Zero
    AND
    Total Outflow over the next timestep > Allowed Fraction *
    Current Volume
Then
    Timestep = (Allowed Fraction * Current Volume)/Rate of
    Volume Change
Else
    Timestep = Default Timestep
  
```



**Note:** Not that even if the two conditions are met, the timestep may not necessarily be shortened. For example, if the outflow was large but the inflow was also large (but not equal to the outflow), the Rate of Volume Change would be small, and the computed timestep could be larger than the default timestep (i.e., the timestep would not be shortened and the default timestep would be used). This, of course, is what we want. We do not want to shorten the timestep unless it is required to improve accuracy.

Assuming that the volume of the Cell that we are concerned with is computed using a Pool element (named, for example, **Volume1**), we could then define an Expression (**MaxStep1**) that defines the maximum allowable timestep as follows:

```

if(Abs(Net_Out) > 0 m3/day and Volume1.Total_Outflow* Default_DT /
Volume1>Allowed_Fraction, Allowed_Fraction*Volume1/abs(Net_Out),
Default_DT)
  
```

In this equation, **Net\_Out** is simply the total outflow rate minus the total inflow rate:

```

Volume1.Total_Outflow-Volume1.Total_Inflow
  
```



**Note:** A Pool is recommended because it automatically computes the Total\_Inflow and Total\_Outflow.

**Default\_DT** is the default scheduled timestep.



**Note:** If the scheduled timestep was not constant (e.g., you have assigned phases) you would need to define this variable appropriately to represent those phases.

In order for this logic to work, we still must specify a non-zero Lower Bound. And as we will discuss below, we don't want this Lower Bound to be too small (the smaller it is, the shorter the timestep needs to be just before the Cell "empties").

Of course, we could have multiple Cells that may potentially be changing rapidly in this way. In such a case, we would need to compute **MaxStep<sub>n</sub>** for each Cell *n* and then compute **MaxStep** as the minimum of all of these values:

$$\min(\text{MaxStep1}, \text{MaxStep2}, \text{MaxStep3}, \text{MaxStep4})$$

Once this variable is defined, it can simply be entered into the field defining the **Maximum time between updates** in the **Advanced Time Settings** (accessed via the **Time** tab of the Simulation Settings dialog):



GoldSim ensures that the next timestep is no larger than the current value of what is specified in this field (i.e., this represents the maximum timestep allowed). Hence, it only shortens the timestep (it never increases it from the default scheduled timestep). For example, if the default scheduled timestep was 1 day, and **MaxStep** was equal to 0.1 day, GoldSim would shorten the next timestep to 0.1 day. But if **MaxStep** was 10 day, the next timestep would remain at 1 day.

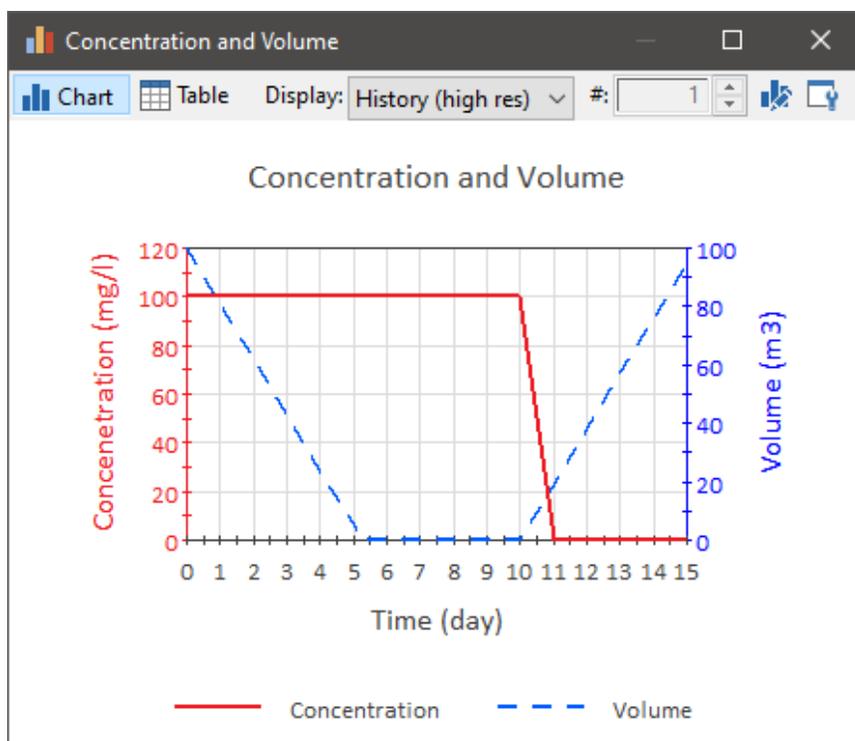


**Note:** Dynamically changing the timestep in this way is discussed in Chapter 7 of the **GoldSim User's Guide**.



**Note:** If your Cells are contained within a Container with an Internal Clock, the **Maximum time between updates** field that should be used is on the **Internal Clock** tab of the Container. Internal Clocks for Containers are also discussed in Chapter 7 of the **GoldSim User's Guide**.

Applying this algorithm to the example problem discussed above with Medium Precision (and an Allowed Fraction of 5%) produces the following result:



This is essentially identical to the Low Precision result (all spikes have been removed). Again, if you wanted to report zero concentration when the Cell was “empty” (at the Lower Bound), you could adjust the concentration when reporting it:

If(Volume = Lower Bound, 0 mg/l, Concentration)

To summarize, the approach to handling rapidly changing Cell volumes (and emptying Cells), that can produce spiky concentrations while maintaining the accuracy improvements of Low and High Precision solutions is as follows:

1. Create a non-zero Lower Bound for the media amounts that are rapidly changing in the Cell (typically the Reference Fluid water, but could be another Fluid, or a Solid if you were simulating advection in these media).
2. Define a maximum timestep allowed for that Cell based on the Cell media amount, and the inflows and outflows of that media. For example:

```
if(Abs(Net_Out) > 0 m3/day and Volume1.Total_Outflow*
Default_DT / Volume1 > Allowed_Fraction,
Allowed_Fraction*Volume1/abs(Net_Out), Default_DT)
```

The Allowed Fraction is the maximum allowable fractional change that appropriately minimizes the error. GoldSim provides a warning message if the fractional change is greater than 10%. For many systems, the fractional change will likely need to be higher than this to produce a significant error, but the warning is conservatively displayed at 10%. Experimentation will be required to determine the appropriate value. You want to use the largest value that minimizes the error to an acceptable level.

3. If there are multiple Cells that may potentially be changing rapidly in this way, compute the maximum timestep allowed for each Cell and then compute the minimum of these values.
4. Enter this value into the field defining the **Maximum time between updates** in the **Advanced Time Settings** (accessed via the **Time** tab of the Simulation Settings dialog).

This algorithm works very well and is generally very efficient (the timestep is only minimized rarely and when it needs to be).

The two parameters that control the accuracy are the Allowed Fraction and the Lower Bound. The smaller these values, the smaller the error. Of course, as these values are reduced, the timestep becomes smaller (and the computational effort increases). As a result, some experimentation may be required to determine the most appropriate values for a particular system. As pointed out above, for most systems, the fractional change will likely need to be greater than 20% or so to produce a significant error. Of course, a larger Lower Bound also results in more mass left behind in an “empty” Cell, but in many cases, this may not pose a problem (e.g., it quickly re-enters the system when the Cell refills).

The higher the net outflow (Net\_Out above) as the volume approaches zero, the greater number of timesteps that will be required (e.g., the smaller Allowed Fraction may need to be). It should be noted, however, that in the real-world, outflow rates generally decrease as the volume decreases (due to natural feedback loops). For example, as the volume of a pond decreases, the surface area of the pond decreases, and the evaporation rate decreases. Similarly, as a pond volume decreases, the pumping rate will often be lowered (e.g., either by turning off one of several pumps or adjusting the pumping rate of variable speed pumps). These kinds of feedback loops result in a more gradual approach to the Lower Bound (and it is strongly recommended that you represent them in your model if they are present).

## Pipe Pathway Details

The governing equations for Pipe pathways and the manner in which these equations are solved by GoldSim are discussed below.

### Governing Equations for Pipe Pathways

Within GoldSim, we are primarily interested in computing the flux of each species leaving the pathway as a function of time. This can be expressed as a function of the (dissolved plus sorbed onto suspended solids) concentration of the species in the flowing (reference) fluid at the end of the pathway.

$$\text{Flux}_s = \left( Q \cdot SV_s \cdot c_{m,s} - (A_m D_s + \alpha \cdot Q \cdot SV_s) \frac{\partial c_{m,s}}{\partial x} \right) \Bigg|_{x=L} \quad (\text{B-25})$$

where:

- Flux<sub>s</sub> = flux of species s leaving the pathway (M/T);
- Q = volumetric flow rate of fluid in the pathway (L<sup>3</sup>/T);
- SV<sub>s</sub> = suspended solid velocity magnification factor for species s.
- c<sub>m,s</sub> = mean mobile concentration of species s in available fraction of saturated pore space in mobile zone of pathway (M/L<sup>3</sup>);
- A<sub>m</sub> = cross-sectional area of the mobile zone (L<sup>2</sup>);

$D_s$	=	effective diffusivity of species $s$ in the mobile zone $= n_{m,s} t_m d_{m,r} d_{m,s}$
$n_{m,s}$	=	available porosity of the porous medium in the mobile zone for species $s$ ;
$t_m$	=	tortuosity of the infill material
$d_{m,r}$	=	reference diffusivity for the reference fluid
$d_{m,s}$	=	relative diffusivity for species $s$ in the reference fluid
$\alpha$	=	dispersivity of the pathway (L);
$L$	=	length of the pathway (L);
$x$	=	distance into the pathway (L); and



**Note:** The tortuosity is defined in different ways in different fields. Within GoldSim, it is defined such that the smaller the tortuosity, the more tortuous the path. In some fields, the tortuosity is defined as the inverse of how it is defined in GoldSim, such that more tortuous paths have a *higher* Tortuosity.

The suspended solid velocity magnification factor accounts for the effective increase in the mass flux due to the presence of suspended solids in the mobile fluid, and is defined as follows. Note that we ignore diffusion of suspended solids:

$$SV_s = \frac{1 + c_{ss} \cdot vm_{ss} \cdot K_{ss,s}}{1 + c_{ss} \cdot K_{ss,s}} \quad (B-26)$$

where:

$c_{ss}$	=	concentration of the suspended solid in the mobile zone (M/L <sup>3</sup> );
$vm_{ss}$	=	the advective velocity multiplier for suspended solid; and
$K_{ss,s}$	=	partition coefficient between the suspended solid and the reference fluid for species $s$ (L <sup>3</sup> /M).

### Concentration of Species in the Mobile Zone

In order to compute the flux of species leaving the pathway, it is first necessary to compute the concentration of the species in the mobile zone of the pathway. The governing equation for the concentration in the mobile zone of a pipe is as follows:

$$\begin{aligned} \frac{\partial c_{ms}}{\partial t} = & - \left[ \left( \frac{Q \cdot SV_s}{n_{ms} A_m R_{ms}} \right) \frac{\partial c_{ms}}{\partial x} - \left( \frac{A_m D_s + \alpha Q \cdot SV_s}{n_{ms} A_m R_{ms}} \right) \frac{\partial^2 c_{ms}}{\partial x^2} \right] \\ & + \left[ -c_{ms} \lambda_s + \sum_{p=1}^{NP_s} c_{m,p} \lambda_p f_{ps} S_{ps} \left( \frac{AW_s}{AW_p} \right) \left( \frac{R_{m,p}}{R_{ms}} \right) \left( \frac{n_{m,p} SF_p}{n_{ms} SF_s} \right) \right] \\ & - \left[ \frac{F_{st,s}}{n_{ms} A_m R_{ms}} \right] \end{aligned} \quad (B-27)$$

where:

$A_m$	=	cross-sectional area of the mobile zone ( $L^2$ );
$R_{m,s}$	=	retardation factor for species $s$ in the mobile zone. Defined in Equation B-30, this is the ratio of mobile to total mass in the mobile zone;
$R_{m,p}$	=	retardation factor for species $p$ in the mobile zone;
$\lambda_s$	=	decay rate for species $s$ ( $T^{-1}$ );
$\lambda_p$	=	decay rate for parent species $p$ ( $T^{-1}$ );
$f_{ps}$	=	fraction of parent $p$ which decays into species $s$ ;
$NP_s$	=	number of direct parents of species $s$ ;
$S_{ps}$	=	stoichiometric ratio of moles of species $s$ produced per mole of species $p$ which decays;
$AW_s$	=	molecular (or atomic) weight of species $s$ (M/mole);
$AW_p$	=	molecular (or atomic) weight of parent species $p$ (M/mole);
$n_{m,p}$	=	available porosity of the porous medium in the mobile zone for species $p$ ;
$n_{m,s}$	=	available porosity of the porous medium in the mobile zone for species $s$ ;
$c_{m,p}$	=	dissolved concentration of parent species $p$ in mobile zone of pathway ( $M/L^3$ );
$F_{st,s}$	=	flux of species $s$ from the mobile zone to storage zones per unit length of pathway ( $M/T/L$ );
$SF_p$	=	Suspended solid storage factor for species $p$ ; and
$SF_s$	=	Suspended solid storage factor for species $s$ .

and

$$SF_i = 1 + c_{ss} \cdot K_{ss,i} \quad (B-27a)$$

where

$c_{ss}$	=	concentration of the suspended solid in the mobile zone ( $M/L^3$ );
$K_{ss,i}$	=	partition coefficient between the suspended solid and the reference fluid for species $i$ ( $L^3/M$ ).

$SF_i$  represents the ratio of mobile to dissolved mass in the mobile zone.

Note that the available porosity for species  $s$  in the mobile zone porous medium,  $n_{m,s}$ , is defined as  $f_{ms} n_m$ , where  $n_m$  is the actual porosity of the solid in the mobile zone of the pipe, and  $f_{ms}$  is the available porosity of the mobile zone porous medium for species  $s$ .

Equation (B-27) is simply an expanded version of the one-dimensional advection-dispersion equation. The first term in the right-hand side of the equation represents the rate of change due to advective and dispersive fluxes; the second term represents the rate of change due to decay and ingrowth; and the third term represents the rate of change due to exchanges with storage zones. Note that the solutions for the concentration of each species in a decay chain are

coupled with the other members of the decay chain (through the ingrowth terms), and hence they must be solved as a coupled system of equations.

The boundary conditions for equation (B-27) are as follows:

- $c_{m,s} \rightarrow 0$  as  $x \rightarrow \infty$ ; and
- at  $x = 0$ , a flux boundary condition is applied such that:

$$\left( QSV_s c_{m,s} - (A_m D_s + \alpha QSV_s) \frac{\partial c_{m,s}}{\partial x} \right) \Big|_{x=0} = \delta(t) M_{init,s} + F_{bc,s} + F_{paths,s} \quad (B-28)$$

where:

- $M_{init,s}$  = user-specified initial mass of species  $s$  applied to the pathway (M);
- $F_{bc,s}$  = user-specified boundary flux for species  $s$  (M/T);
- $F_{paths,s}$  = flux of species  $s$  into pathway from other GoldSim pathways (M/T); and
- $\delta(t)$  = the Dirac delta function ( $T^{-1}$ ).

The flux from other pathways is specified indirectly by the user by creating an advective or diffusive mass flux link from one or more pathways to the pipe.

With the exception of  $A_m$ ,  $R_{m,s}$ ,  $R_{m,p}$ , and  $F_{st,s}$ , all of the parameters in the equations presented above are directly specified by the user in GoldSim.

$A_m$  represents the cross-sectional area of the mobile zone. It is computed as follows:

$$A_m = A_t (1 - f_{stag}) \quad (B-29)$$

where:

- $A_t$  = the total area of the pathway ( $L^2$ ); and
- $f_{stag}$  = the fraction of the pathway area associated with a stagnant zone.

$A_t$  and  $f_{stag}$  are specified directly by the user.

The retardation factor for the mobile zone accounts for the influence of any porous medium that may exist in the pathway, as well as the influence of particulates, partial saturation, and any coating along the perimeter of the pathway. It is the ratio of the total mass of species  $s$  to the mobile mass (dissolved plus sorbed onto suspended solids):

$$R_{m,s} = \frac{PT(\rho_c K_{c,s} + n_{c,s}) + A_m(\rho_p K_{p,s} + n_{m,s} SF_s \theta)}{A_m n_{m,s} SF_s \theta} \quad (B-30)$$

where:

- $R_{m,s}$  = retardation factor for species  $s$  in the mobile zone;
- $P$  = perimeter of the pathway (L);
- $T$  = thickness of the coating (L);
- $A_m$  = cross-sectional area of the mobile zone ( $L^2$ );

- $\rho_c$  = dry bulk density of the coating material ( $M/L^3$ );
- $\rho_p$  = dry bulk density of the porous infill material ( $M/L^3$ );
- $n_{c,s}$  = available porosity of the coating material for species  $s$ ;
- $\theta$  = fluid saturation of the available pores in the mobile zone;
- $SF_s$  = suspended solid storage factor;
- $K_{c,s}$  = partition coefficient for species  $s$  in the coating material ( $L^3/M$ ); and
- $K_{p,s}$  = partition coefficient for species  $s$  in the porous infill material ( $L^3/M$ ).

and

$$SF_s = 1 + c_{ss} \cdot K_{ss,s} \quad (B-30a)$$

where

- $c_{ss}$  = concentration of the suspended solid in the mobile zone ( $M/L^3$ );
- $K_{ss,s}$  = partition coefficient between the suspended solid and the reference fluid for species  $s$  ( $L^3/M$ ).

Note that the available porosity for species  $s$  in the coating material,  $n_{c,s}$ , is defined as  $f_{cs} n_c$ , where  $n_c$  is the actual porosity of the solid in the coating material, and  $f_{cs}$  is the available porosity of the coating material solid for species  $s$ .

This equation reduces to the standard form for a retardation factor if the thickness of the coating is equal to zero and no suspended solids are present.

The  $F_{st,s}$  term represents the flux of species  $s$  into storage zones (per unit length), and is made up of two terms:

$$F_{st,s} = F_{md,s} + F_{sd,s} \quad (B-31)$$

where:

- $F_{md,s}$  = total flux of species  $s$  into matrix diffusion zones per unit length of pathway ( $M/T/L$ ); and
- $F_{sd,s}$  = flux of species  $s$  into a stagnant dispersive zone per unit length of pathway ( $M/T/L$ ).

$F_{md,s}$  is defined as follows:

$$F_{md,s} = - \sum_{im=1}^{NMD} P f_{im} D_{im,s} \left. \frac{\partial c_{im,s}}{\partial z} \right|_{z=0} \quad (B-32)$$

where:

- $P$  = perimeter of the pathway ( $L$ );
- $f_{im}$  = fraction of perimeter associated with matrix diffusion zone  $im$ ;
- $D_{im,s}$  = diffusivity of matrix diffusion zone  $im$  for species  $s$  ( $L^2/T$ );

- $c_{im,s}$  = concentration of species s in matrix diffusion zone im of pathway ( $M/L^3$ );
- NMD = the number of matrix diffusion zones; and
- $z$  = distance in the matrix diffusion zone (L).

Note that in this equation, the  $z$  axis is orthogonal to the flow direction in the pathway, with  $z = 0$  representing the boundary between the mobile zone and the matrix diffusion zone.

$F_{sd,s}$  is defined as follows:

$$F_{sd,s} = \beta SF_s Q (c_{m,s} - c_{sd,s}) \quad (B-33)$$

where:

- $\beta$  = probability of an individual solute molecule moving from the mobile zone to the stagnant zone, per length of distance traveled in the mobile zone ( $L^{-1}$ );
- $Q$  = volumetric flow rate of fluid in the pathway ( $L^3/T$ );
- $c_{m,s}$  = Concentration of species s in the mobile zone fluid ( $M/L^3$ );
- $SF_s$  = Suspended solid magnification factor for species s; and
- $c_{sd,s}$  = concentration of species s in stagnant dispersive zone of pathway ( $M/L^3$ ).

Note that neither  $F_{md,s}$  nor  $F_{sd,s}$  are functions of the suspended solids concentration, since suspended solids are assumed not to interact with the storage zones.

As can be seen, both  $F_{md,s}$  and  $F_{sd,s}$  are functions of the species concentrations in the storage zones. Hence, in order to compute these flux terms, it is necessary to couple the equations for the concentrations in the storage zones with that for the concentration of the species in the mobile zone of the pathway.

The governing equation for the concentration in a matrix diffusion zone of a pipe pathway is as follows:

**Concentration of Species in the Matrix Diffusion Zone(s)**

$$\frac{\partial c_{im,s}}{\partial t} = \left[ \left( \frac{D_{im,s}}{n_{im,s} R_{im,s}} \right) \frac{\partial^2 c_{im,s}}{\partial z^2} + \left( \frac{D_{im,s}}{n_{im,s} A_{im} R_{im,s}} \right) \frac{\partial A_{im}}{\partial z} \frac{\partial c_{im,s}}{\partial z} \right] + \left[ -c_{im,s} \lambda_s + \sum_{p=1}^{NP_s} c_{im,p} \lambda_p f_{ps} S_{ps} \left( \frac{AW_s}{AW_p} \right) \left( \frac{R_{im,p}}{R_{im,s}} \right) \left( \frac{n_{m,p} SF_p}{n_{m,s} SF_s} \right) \right] \quad (B-34)$$

where:

- $c_{im,s}$  = concentration of species s in matrix diffusion zone im ( $M/L^3$ );
- $D_{im,s}$  = diffusivity of species s in matrix diffusion zone ( $L^2/T$ );
- $n_{im,s}$  = Available porosity of the porous medium in the matrix diffusion zone for species s;

$A_{im}$	=	diffusive area of the matrix diffusion zone per unit length of mobile zone (L); $A_{im}(z=0) = Pf_{im}$
$R_{im,s}$	=	retardation factor for species s in the matrix diffusion zone;
$R_{im,p}$	=	retardation factor for species p in the matrix diffusion zone
$\lambda_s$	=	decay rate for species s ( $T^{-1}$ );
$\lambda_p$	=	decay rate for parent species p ( $T^{-1}$ );
$f_{ps}$	=	fraction of parent p which decays into species s;
$NP_s$	=	number of direct parents of species s;
$S_{ps}$	=	stoichiometric ratio of moles of species s produced per mole of species p which decays;
$AW_s$	=	molecular (or atomic) weight of species s (M/mole);
$AW_p$	=	molecular (or atomic) weight of parent species p (M/mole);
$c_{im,p}$	=	concentration of parent species p in mobile zone of pathway ( $M/L^3$ ).
$n_{m,p}$	=	available porosity of the porous medium in the mobile zone for species sp;
$n_{m,s}$	=	available porosity of the porous medium in the mobile zone for species s;
$SF_p$	=	Suspended solid storage factor for species p; and
$SF_s$	=	Suspended solid storage factor for species s.

and

$$SF_i = 1 + c_{ss} \cdot K_{ss,i} \quad (B-34a)$$

where

$c_{ss}$	=	concentration of the suspended solid in the mobile zone ( $M/L^3$ );
$K_{ss,i}$	=	partition coefficient between the suspended solid and the reference fluid for species i ( $L^3/M$ ).

Note that the available porosity for species s in the matrix diffusion zone material,  $n_{im,s}$ , is defined as  $f_{ims} n_{im}$ , where  $n_{im}$  is the actual porosity of the solid in the matrix diffusion zone, and  $f_{ims}$  is the available porosity of the matrix diffusion zone solid for species s.

In this equation, the z axis is orthogonal to the flow direction in the pathway, with  $z = 0$  representing the boundary between the mobile zone and the matrix diffusion zone.

The first term in the equation represents the rate of change due to diffusive fluxes. The second term represents the rate of change due to decay and ingrowth. Note that the solutions for the concentration of each species in a decay chain are coupled with the other members of the decay chain (through the ingrowth terms), and hence they must be solved as a coupled system of equations.

GoldSim allows up to three matrix diffusion zones to be specified, as well as a “skin” zone. The three matrix diffusion zones exist in parallel. The skin zone, if present, is assumed to be present in front of all matrix diffusion zones (i.e., between the matrix diffusion zones and the mobile zone). Hence, if a skin zone is present, species must first diffuse through the skin before reaching the underlying diffusive zones (forming a two-layer diffusive system). Equation (B-34) is applied individually to the three matrix diffusion zones and the skin.

The inner boundary condition (at  $z=0$ , closest to the mobile zone) for the skin zone, if present, and for the matrix diffusion zones (in the absence of skin) is :

$$c_{im,s} = c_{m,s} \quad \text{at } z=0 \quad (\text{B-35})$$

The outer boundary condition for the matrix diffusion zones (or the skin in the absence of matrix diffusion zones) is:

$$\frac{\partial c_{im,s}}{\partial z} = 0 \quad \text{at } z=T_{im} \quad (\text{B-36})$$

where  $T_{im}$  is the thickness of the diffusion zone.

The outer boundary condition for the skin (in the presence of other matrix diffusion zones) is:

$$D_{skin,s} \frac{\partial c_{skin,s}}{\partial z_{skin}} = \sum_{im=1}^{NMD} f_{im} D_{im,s} \frac{\partial c_{im,s}}{\partial z_{md}} \Bigg|_{z_{md}=0} \quad \text{at } z_{skin} = T_{skin} \quad (\text{B-37})$$

where:

- $c_{skin,s}$  = concentration of species  $s$  in the skin zone of pathway ( $M/L^3$ );
- $c_{im,s}$  = concentration of species  $s$  in matrix diffusion zone  $im$  of pathway ( $M/L^3$ );
- $f_{im}$  = fraction of perimeter associated with matrix diffusion zone  $im$ ;
- $D_{skin,s}$  = diffusivity of skin zone for species  $s$  ( $L^2/T$ );
- $D_{im,s}$  = diffusivity of matrix diffusion zone  $im$  for species  $s$  ( $L^2/T$ );
- $NMD$  = the number of matrix diffusion zones; and
- $T_{skin}$  = thickness of skin zone ( $L$ ).

This boundary condition couples the skin equation to the matrix diffusion zone equations by setting the total flux into the matrix diffusion zones equal to the flux out of the skin. (Both  $z_{md}$  and  $z_{skin}$  represent axes orthogonal to the direction of flow.  $z_{skin}$  is the axis relative to the skin,  $z_{md}$  is the axis relative to the matrix diffusion zones. That is,  $z_{skin} = 0$  at the interface between the mobile zone and the skin, whereas  $z_{md} = 0$  at the interface between the skin and the matrix diffusion zones.)

$A_{im}$  represents the diffusive area (per unit length of the pathway). It is a function of the assumed geometry of diffusion, and hence varies with distance ( $z$ ):

$$A_{im} = P f_{im} f(z) \quad (\text{B-38})$$

where  $f(z)$  is a function which depends on the specified geometry. GoldSim provides three options for the assumed geometry for diffusion:

$$\begin{aligned} \text{Slab (constant):} & \quad f(z) = 1 \\ \text{Sphere:} & \quad f(z) = (T_{im} - z)^2 \\ \text{Slot (exponential):} & \quad f(z) = e^{2z} \quad (z \text{ in meters}) \end{aligned}$$

Note that the geometry of the skin zone is always assumed to be “Slab”.

The retardation factor for the matrix diffusion zones and the skin is computed as follows:

$$R_{im,s} = 1 + \frac{\rho_{im} K_{im,s}}{n_{im,s}} \quad (\text{B-39})$$

where:

$$\begin{aligned} R_{im,s} &= \text{retardation factor for species } s \text{ in the matrix diffusion zone;} \\ \rho_{im} &= \text{dry bulk density of the porous material in the matrix diffusion zone (M/L}^3\text{);} \\ n_{im,s} &= \text{available porosity of the material in the matrix diffusion zone for species } s; \\ K_{im,s} &= \text{partition coefficient for species } s \text{ in the porous material in the matrix diffusion zone (L}^3\text{/M).} \end{aligned}$$

The diffusivity ( $D_{im,s}$ ) is computed as a function of the properties of the fluid medium and the solid porous medium through which the species is diffusing:

$$D_{im,s} = n_{im,s} t_{im} d_{im,r} d_{im,s} \quad (\text{B-40})$$

where:

$$\begin{aligned} D_{im,s} &= \text{effective diffusivity of species } s \text{ in matrix diffusion zone } im \text{ (L}^2\text{/T);} \\ n_{im,s} &= \text{available porosity of the material in matrix diffusion zone } im \text{ for species } s; \\ t_{im} &= \text{tortuosity of the material in matrix diffusion zone } im; \\ d_{im,r} &= \text{reference diffusivity for the fluid in matrix diffusion zone } im \text{ (L}^2\text{/T);} \text{ and} \\ d_{im,s} &= \text{relative diffusivity for species } s \text{ within the fluid in matrix diffusion zone } im. \end{aligned}$$

Note that the user does not define a single value for the thickness of each matrix diffusion zone. Rather, a minimum and maximum thickness is specified. GoldSim assumes that along the pathway, the thickness of the zone varies randomly between these two extremes, such that every part of the pathway perimeter “sees” the full range of matrix thicknesses.

Mathematically, this is represented in GoldSim by integrating the flux for each of the matrix diffusion zones over the specified range of thickness. That is, equation (B-32) is actually computed by GoldSim as follows:

$$F_{md,s} = \sum_{im=1}^{NMD} \left[ \int_{\tau=T_{im,min}}^{T_{im,max}} \frac{P f_{im} D_{im,s}}{(T_{im,max} - T_{im,min})} \left( \frac{\partial c_{im,s}(\tau)}{\partial z} \Big|_{z=0} \right) \delta\tau \right] \quad (B-41)$$

where:

- $F_{md,s}$  = total flux of species s into matrix diffusion zones per unit length of pathway (M/T/L);
- $P$  = perimeter of the pathway (L);
- $f_{im}$  = fraction of perimeter associated with matrix diffusion zone im;
- $D_{im,s}$  = diffusivity of matrix diffusion zone im for species s ( $L^2/yr$ );
- $c_{im,s}(\tau)$  = concentration of species s in a matrix diffusion zone im of thickness  $\tau$  ( $M/L^3$ );
- $T_{im,min}$  = minimum thickness of matrix diffusion zone im (L);
- $T_{im,max}$  = maximum thickness of matrix diffusion zone im (L); and
- $NMD$  = the number of matrix diffusion zones.

**Concentration of Species in the Stagnant Dispersive Zone**

The governing equation for the concentration in the stagnant dispersive zone of a one-dimensional pathway is as follows:

$$\frac{\partial c_{sd,s}}{\partial t} = - \left[ \frac{\beta Q S V_s}{f_{stag} n_{sd,s} R_{sd,s}} (c_{m,s} - c_{sd,s}) \right] + \left[ -c_{sd,s} \lambda_s + \sum_{p=1}^{NP_s} c_{sd,p} \lambda_p f_{ps} S_{ps} \left( \frac{AW_s}{AW_p} \right) \left( \frac{R_{sd,p}}{R_{sd,s}} \right) \left( \frac{n_{m,p} SF_p}{n_{m,s} SF_s} \right) \right] \quad (B-42)$$

where:

- $\beta$  = probability of an individual solute molecule (or suspended particle) moving from the mobile zone to the stagnant zone, per unit of distance traveled in the mobile zone ( $L^{-1}$ );
- $Q$  = volumetric flow rate of fluid in the pathway ( $L^3/T$ );
- $SV_s$  = suspended solid magnification factor for species s (see Equation B-26);
- $c_{m,s}$  = concentration of species s in mobile zone of pathway ( $M/L^3$ );
- $c_{sd,s}$  = concentration of species s in stagnant dispersive zone of pathway ( $M/L^3$ );
- $f_{stag}$  = the fraction of the pathway area associated with a stagnant zone;
- $n_{sd,s}$  = available porosity of the porous medium in the stagnant dispersive zone for species s;
- $R_{sd,s}$  = retardation factor for species s in the stagnant dispersive zone;

$R_{sd,p}$	=	retardation factor for parent species p in the stagnant dispersive zone;
$\lambda_s$	=	decay rate for species s ( $T^{-1}$ );
$\lambda_p$	=	decay rate for parent species p ( $T^{-1}$ );
$f_{ps}$	=	fraction of parent p which decays into species s;
$NP_s$	=	number of direct parents of species s;
$S_{ps}$	=	stoichiometric ratio of moles of species s produced per mole of species p which decays;
$AW_s$	=	molecular (or atomic) weight of species s (M/mole);
$AW_p$	=	molecular (or atomic) weight of parent species p (M/mole);
$c_{sd,p}$	=	concentration of parent species p in stagnant dispersive zone of pathway ( $M/L^3$ ).
$n_{m,p}$	=	available porosity of the porous medium in the mobile zone for species sp;
$n_{m,s}$	=	available porosity of the porous medium in the mobile zone for species s;
$SF_p$	=	Suspended solid storage factor for species p; and
$SF_s$	=	Suspended solid storage factor for species s.

and

$$SF_1 = 1 + c_{ss} \cdot K_{ss,i} \quad (B-42a)$$

where

$c_{ss}$	=	concentration of the suspended solid in the mobile zone ( $M/L^3$ );
$K_{ss,i}$	=	partition coefficient between the suspended solid and the reference fluid for species i ( $L^3/M$ ).

Note that the solutions for the concentration of each species in a decay chain are coupled with the other members of the decay chain (through the ingrowth terms), and hence must be solved as a coupled system of equations.

The retardation factor for the stagnant dispersive zone is computed as follows:

$$R_{sd,s} = \frac{\rho_{sd} K_{sd,s} + n_{sd,s} SF_s}{n_{sd,s} SF_s} \quad (B-43)$$

where:

$R_{sd,s}$	=	retardation factor for species s in the stagnant dispersive zone;
$\rho_{sd}$	=	dry bulk density of the porous material in the stagnant dispersive zone ( $M/L^3$ );
$n_{sd,s}$	=	available porosity of the material in the stagnant dispersive zone for species s;
$K_{sd,s}$	=	partition coefficient for species s in the porous material in the stagnant dispersive zone ( $L^3/M$ ); and

## Solution Technique for Pipe Pathways

$SF_s$  = suspended solid magnification factor for species  $s$  (see Equation B-26).

GoldSim solves the Pipe pathway equations using Laplace transforms. The central concept of the Laplace transform solution technique is that for an advectively-dominated system, the discharge history is a linear function of the input history.

The *transfer function* for a pathway is defined as its discharge history resulting from a unit slug input at time  $t=0$ . Because of chain decay, the resulting transfer function for each input species is actually a vector, as there will be discharge histories for the species itself and also for its descendants. Considering inputs from all members of a decay chain, the result is a transfer function matrix  $\mathbf{T} = [t_{rc}]$ , where  $t_{rc}$  is the pathway's discharge rate of species  $r$  due to a unit input of species  $c$  at time 0. For convenience, it is assumed that parents always precede children in the arrays, so that  $\mathbf{T}$  is lower-triangular in form.

The discharge history at the end of the pathway,  $x=L$ , is therefore expressed as a convolution integral:

$$\mathbf{f}(L, t) = \int_0^t \mathbf{f}(0, \tau) \mathbf{T}(t - \tau) d\tau \quad (\text{B-44})$$

where  $\mathbf{f}$  is a vector containing the flux of each species in the decay chain.

Note that in the above equation,  $\mathbf{T}$  is a matrix whose entries are themselves functions of time (i.e., discharge histories due to slug inputs of each species in the decay-chain).

The Laplace transform of the convolution integral has a very simple form:

$$\mathbf{f}^*(L) = \mathbf{T}^* \mathbf{f}^*(0) \quad (\text{B-45})$$

where the transformed transfer matrix  $\mathbf{T}^*$  is a matrix of complex numbers, which are functions of the Laplace variable  $s$ , and the transformed influx vector  $\mathbf{f}^*(0)$  is the Laplace transform of the pathway mass influx history.

GoldSim models each pipe pathway by calculating the Laplace transform,  $\mathbf{T}^*$ , of the transfer function matrix for the mass discharge rate  $\mathbf{f}^*(L)$ . At each timestep, changes to input rates to the Pipe pathway are Laplace-transformed (assuming they are step-functions as of the previous GoldSim timestep), multiplied by the transfer matrix, and summed. In this way, GoldSim maintains an  $\mathbf{f}^*(L)$  buffer with the transformed discharge fluxes for the pathway.

At each step, GoldSim calculates the incremental discharges from the Pipe pathways during the step, which are then passed on to the next pathway. The Laplace transform for the incremental pathway discharge is computed as follows:

$$\int_{t-\Delta t}^t \mathbf{f}(L, \tau) d\tau = \int_0^t [\mathbf{f}(L, \tau) - \mathbf{f}(L, \tau - \Delta t)] d\tau = L^{-1} \left\{ \frac{1 - e^{-s\Delta t}}{s} \mathbf{f}^*(L) \right\} \quad (\text{B-46})$$

where:

$\mathbf{f}$  = flux in the pathway (M/T);  
 $L$  = length of the pathway (L)  
 $\Delta t$  = GoldSim timestep (T); and

$L^{-1}$  = the inverse Laplace transform.

The discharge flux is calculated by numerically inverting the transformed discharge, using the de Hoog algorithm (de Hoog et al., 1982). There are numerous other algorithms for Laplace inversion (notably Talbot's method), but an evaluation of Talbot's method found the de Hoog method was superior to it in terms of reliability, accuracy and efficiency. GoldSim's implementation of the de Hoog algorithm uses a technique developed by Prof. Edward Sudicky at the University of Waterloo, where a separate set of s-values is used to do the transformations and inversions for each factor of ten in the time domain.

A 'basic time step'  $\Delta t$  is defined as the greater of the first scheduled timestep for the model and the total simulation time divided by the maximum allowable number of basic time steps. The maximum number is  $10^5$  for low-precision solutions,  $10^6$  for medium-precision, and  $10^8$  for high-precision.

Within the de Hoog algorithm,  $2 \cdot N_{\text{term}} + 1$  s-values are used per factor of ten in the time domain (e.g., from  $\Delta t$  to  $10 \Delta t$ , and from  $10 \Delta t$  to  $100 \Delta t$ , etc.). The value of  $N_{\text{term}}$  is controlled by the user-selected solution precision option. A precision setting of Low gives  $N_{\text{term}}=5$ , Medium gives  $N_{\text{term}}=15$ , and High gives  $N_{\text{term}}=25$ . The user is advised to test their system by applying a step-function of mass, and confirming that the resulting discharge history is smooth. An insufficient value of  $N_{\text{term}}$  will typically result in oscillations about the mean value of the calculated result.

(The de Hoog algorithm also has a second control parameter which represents the internal accuracy to which the Laplace transforms have been calculated. The default value of 1E-12 appears to give reliable results, and cannot be modified by the user.)

Note that if the system properties change at some point in time, GoldSim is not able to modify the existing array of transformed cumulative discharges, which represents the predicted discharge histories for species which are already in the pathway. However, GoldSim does update the transfer matrix, so that future inputs to the pathway will have their discharges calculated using the updated transfer matrix.

### **Pipe Solution Technique Notation**

The notation system used in this section is summarized below:

- Matrices are displayed in bold, capitals: **M**, or in brackets as  $[m_{rc}]$ , where  $m_{rc}$  is the entry in row r, column c of the matrix.
- Diagonal matrices are displayed as  $[m_r]$ . Vectors are displayed in bold, lower-case: **v**, or in braces as  $\{v_r\}$ , where  $v_r$  is entry r in the vector.
- Laplace transforms of quantities are expressed with a superscripted asterisk:  $\mathbf{c}^*$ , and the Laplace variable is defined as s.
- Where a local eigenvector-based coordinate system is used to derive a solution to the governing transport equations, values expressed in that coordinate system are shown underlined, e.g.,  $\underline{c}$ .

The mathematical operations derived below contain numerous matrix operations. The user should note that because all of the matrices used are either diagonal or lower-triangular, matrix operations such as inversion and solution of eigenvectors are greatly simplified.

Note that GoldSim solves the equations for Pipe pathways one decay chain at a time, and all of the following discussions refer to a single decay chain.

### Mathematical Representation of the Mobile Zone

The general solution for the transfer matrix of a Pipe pathway is developed in this section, for a mobile zone with an arbitrary number and type of storage zones. This is accomplished by referring to a generic interchange flux of species between the flowing zone and the storage zones, using transfer matrices  $\mathbf{X}_z$  to express the fluxes from the mobile zone to the storage zones.

**Read more:** [Mathematical Representation of Matrix Diffusion Zones](#) (page 364); [Mathematical Representation of Stagnant Dispersive Zone](#) (page 371).

### Mobile Zone: Governing Equation

The following symbols are used in this section:

$\alpha$	=	pathway dispersivity (L);
$\upsilon$	=	an eigenvalue of the $\mathbf{M}$ matrix;
$A$	=	cross-sectional area of the flowing zone ( $L^2$ );
$a_r$	=	coefficient used in the solution;
$b_r$	=	coefficient used in the solution;
$\mathbf{c}$	=	vector of mean mobile species concentrations in the flowing pores, with parents preceding daughters ( $M/L^3$ ), includes dissolved mass plus mass sorbed onto suspended solids;
$\mathbf{c}'$	=	$\partial \mathbf{c} / \partial x$ , the first derivative of $\mathbf{c}$ with respect to distance $x$ ( $M/L^4$ );
$\mathbf{c}''$	=	$\partial^2 \mathbf{c} / \partial x^2$ , the second derivative of $\mathbf{c}$ with respect to distance $x$ ( $M/L^5$ );
$d$	=	dispersion coefficient = $\alpha q$ ( $L^2/T$ );
$\delta$	=	vector of effective diffusion coefficients ( $L^2T^{-1}$ );
$\mathbf{D}$	=	matrix of decay/ingrowth rate factors ( $T^{-1}$ );
$\mathbf{f}$	=	vector of mass fluxes in the $x$ direction ( $M/T$ );
$\mathbf{G}$	=	diagonal matrix of suspended solid storage magnification factors (see Equation B-30a), the ratio of mobile to dissolved mass;
$\mathbf{H}$	=	diagonal matrix of suspended solid velocity magnification factors (see Equation B-26);
$L$	=	pathway length (L);
$\mathbf{M}$	=	a matrix used in the solution of the Laplace transformed equations
$\mathbf{N}_a$	=	diagonal matrix of available porosities for the porous medium in the mobile zone;
$\theta$	=	Fluid saturation of pore space in mobile zone;
$q$	=	Darcy flow velocity ( $L/T$ );
$\mathbf{R}$	=	diagonal matrix of the retardation factors in the mobile zone (see Equation B-30 for definition of individual items), the ratio of the total mass in the mobile zone to the mobile mass;
$s$	=	the (complex) Laplace variable;
$\mathbf{V}$	=	a matrix whose columns are the eigenvectors of $\mathbf{M}$ ;

- $\mathbf{v}_r$  = the  $r$ 'th eigenvector of  $\mathbf{M}$ ;  
 $\lambda_r$  = the  $r$ 'th eigenvalue of  $\mathbf{M}$ ;  
 $x$  = the direction of flow;  
 $\mathbf{x}_z$  = rate of transfer of mass from flowing to immobile zone number  $z$  (M/T);  
 $\mathbf{X}_z$  = transfer matrix for fluxes from the flowing zone to storage zone number  $z$  (M/T); and  
 $z$  = number of storage zones for the pathway.

Consider an infinitesimal unit length of the mobile zone with volume  $A$ . Assuming that the solute species are uniformly mixed at each cross section, the concentrations can be expressed as a function of distance along the path,  $x$ . The amount of mobile (dissolved plus particulate-sorbed) mass is  $\theta AN_a \mathbf{c}$ , and the total amount of mass is  $\theta AN_a \mathbf{Rc}$ .

There are five processes which change the amount of mass: decay, advective transport, diffusive transport, dispersive transport, and interchanges with storage zones. The rate of change (increase) of the total mass in the volume due to each process is as follows:

- *Decay.* The rate of change of the total mass due to decay is  $\mathbf{D}\theta AN_a \mathbf{Rc}$ , where  $\mathbf{D}$  is the matrix of decay and ingrowth coefficients.
- *Advective Transport.* The advective mass flux rate is  $Aq\mathbf{Hc}'$ , and therefore the rate of change of the total mass due to advective transport is  $-Aq\mathbf{Hc}'$ .
- *Diffusive Transport.* The diffusive flux rate is  $-A\delta\mathbf{c}'$ , and therefore the rate of change of the total mass due to diffusion is  $A\delta\mathbf{c}''$ .
- *Dispersive Transport.* The dispersive flux rate is  $-Ad\mathbf{Hc}'$ , and therefore the rate of change of the total mass due to dispersion is  $Ad\mathbf{Hc}''$ .
- *Interchanges with Storage Zones.* The rate of transfer of mass from the mobile zone to storage zone number  $z$ , per unit length of the flowing zone, is defined as  $\mathbf{x}_z$ .

The general differential equation for the conservation of mass in the mobile zone is defined as (Rate of change of total mass) = (Rate of change due to decay) + (Rate of change due to fluxes) + (Rate of change due to outflows to storage zones):

$$\theta AN_a \mathbf{R} \frac{\partial \mathbf{c}}{\partial t} = \mathbf{D}\theta AN_a \mathbf{Rc} - Aq\mathbf{Hc}' + A(\delta + d\mathbf{H})\mathbf{c}'' - \sum_z \mathbf{x}_z \quad (\text{B-47})$$

### Mobile Zone: General Solution

Taking the Laplace transform of Equation (B-47) simply results in replacing  $\mathbf{c}$  by  $\mathbf{c}^*$ , and replacing the time-derivative of  $\mathbf{c}$  by  $s\mathbf{c}^*$ :

$$s\theta AN_a \mathbf{Rc}^* = \mathbf{D}\theta AN_a \mathbf{Rc}^* - Aq\mathbf{Hc}^{*'} + A(\delta + d\mathbf{H})\mathbf{c}^{*''} - \sum_z \mathbf{X}_z \mathbf{c}^* \quad (\text{B-48})$$

Note that the transfer from flowing to storage zones is now expressed using a sum of transfer matrices  $\mathbf{X}_z(s)$ , one per storage zone. The equations for  $\mathbf{X}_z$  are presented in subsequent sections.

**Read more:** [Mathematical Representation of Matrix Diffusion Zones](#) (page 364); [Mathematical Representation of Stagnant Dispersive Zone](#) (page 371).

The transformed flux is:

$$\mathbf{f}^* = Aq\mathbf{H}\mathbf{c}^* - A(\delta + d\mathbf{H})\mathbf{c}^* \quad (\text{B-49})$$

There are boundary conditions at  $x=0$  and  $x=\infty$ . At  $x=0$  the incoming flux to the pathway is prescribed as  $\mathbf{f}_0^*$ . At  $x=\infty$  the concentrations are set equal to zero.

Collecting terms from (B-48) in  $\mathbf{c}$ ,  $\mathbf{c}'$  and  $\mathbf{c}''$ , and pre-multiplying by  $\mathbf{H}^{-1}$ , we get:

$$\mathbf{M}\mathbf{c}^* + Aq\mathbf{c}^* - A(\mathbf{H}^{-1}\delta + d)\mathbf{c}^* = \mathbf{0} \quad (\text{B-50})$$

where

$$\mathbf{M} = \mathbf{H}^{-1} \left( [\mathbf{s}\mathbf{I} - \mathbf{D}] \theta \mathbf{A} \mathbf{N}_a \mathbf{R} + \sum_z \mathbf{X}_z \right) \quad (\text{B-51})$$

and  $\mathbf{M}$  is lower-triangular.

The coupled differential equations shown in matrix form in the above equation can be transformed into a set of uncoupled differential equations by means of a coordinate transformation, from the coordinate system defined by the species concentration vector  $\mathbf{c}$  to new coordinates defined by the eigenvectors  $\mathbf{v}_r$  of the  $\mathbf{M}$  matrix.

Because  $\mathbf{M}$  is lower-triangular, its eigenvalues  $v_r$  are equal to its diagonal terms  $m_{rr}$ . Its eigenvectors  $\mathbf{v}_r$ , which are mutually orthogonal, are readily computed by direct substitution into  $[\mathbf{M} - v_r\mathbf{I}]\mathbf{v}_r = \mathbf{0}$ , arbitrarily setting the  $r$ 'th term in  $\mathbf{v}_r$  to 1.0. Note that terms prior to the  $r$ 'th in  $\mathbf{v}_r$  are equal to zero.

In rare circumstances, the eigenvector calculation may fail if two eigenvalues are identical, and one represents the daughter of the other, resulting in an indefinite  $\mathbf{M}$  matrix. Even if the calculation does not fail, the system of equations can be poorly-conditioned, resulting in erroneous calculations. In order to prevent this possibility, GoldSim automatically checks for daughter-species having (non-zero) decay-rates within a factor of 1.0005 of their parents. If this happens, GoldSim assigns the daughter's decay-rate a value equal to 1.0005 times its parent's decay-rate, and writes a warning message to the run log. The error involved is minor, and this warning message can normally be ignored.

### **Mobile Zone: Eigenvector Coordinate Transformation**

The transformation matrix to convert from the concentration coordinate system to the eigenvector coordinate system is  $\mathbf{V}$ , a matrix whose columns are the eigenvectors of  $\mathbf{M}$ .

Define the eigenvector-transformed Laplace-transformed concentrations and fluxes as  $\underline{\mathbf{c}}$  and  $\underline{\mathbf{f}}$ , respectively. Let

$$\text{the concentration} \quad \underline{\mathbf{c}}^* = \mathbf{V}\mathbf{c}^*; \quad \underline{\mathbf{c}} = \mathbf{V}^{-1}\mathbf{c}^* \quad (\text{B-52})$$

$$\text{and the flux} \quad \underline{\mathbf{f}}^* = \mathbf{V}\mathbf{f}^*; \quad \underline{\mathbf{f}} = \mathbf{V}^{-1}\mathbf{f}^* \quad (\text{B-53})$$

Substituting (B-52) into (B-49):

$$\underline{\mathbf{f}} = Aq\underline{\mathbf{H}}\underline{\mathbf{c}} - A(\underline{\boldsymbol{\delta}} + d\underline{\mathbf{H}})\underline{\mathbf{c}}' \quad (\text{B-54})$$

Substituting (B-52) into (B-50), and pre-multiplying by  $\mathbf{V}^{-1}$  gives:

$$\mathbf{V}^{-1}\mathbf{M}\mathbf{V}\underline{\mathbf{c}} + Aq\underline{\mathbf{c}}' - A(\mathbf{H}^{-1}\underline{\boldsymbol{\delta}} + d)\underline{\mathbf{c}}'' = \mathbf{0} \quad (\text{B-55})$$

Recall that by the definition of the eigenvalues,  $\mathbf{M}\mathbf{V} = \mathbf{V}[\mathbf{v}_r]$ . Therefore, the preceding equation becomes:

$$[\mathbf{v}_r]_r \underline{\mathbf{c}} + Aq\underline{\mathbf{c}}' - A(\mathbf{H}^{-1}\underline{\boldsymbol{\delta}} + d)\underline{\mathbf{c}}'' = \mathbf{0} \quad (\text{B-56})$$

The  $[\mathbf{v}_r]$  matrix of eigenvalues in Equation (B-56) is diagonal, so each row of (B-56) represents a separate ordinary differential equation. The next section will develop the solution for an arbitrary member of this set of differential equations. The solution will lead to the eigenvector-transformed transfer matrix for the pathway,  $\underline{\mathbf{T}}$ , where:

$$\underline{\mathbf{f}}(L) = \underline{\mathbf{T}}\underline{\mathbf{f}}(0) \quad (\text{B-57})$$

Substituting  $\mathbf{V}^{-1}\underline{\mathbf{f}}^*$  for  $\underline{\mathbf{f}}$  and pre-multiplying by  $\mathbf{V}$  gives the solution for the transfer matrix in the original coordinate system:

$$\underline{\mathbf{f}}^*(L) = \underline{\mathbf{V}}\underline{\mathbf{T}}\underline{\mathbf{V}}^{-1}\underline{\mathbf{f}}^*(0)$$

i.e.,  $\underline{\mathbf{T}} = \underline{\mathbf{V}}\underline{\mathbf{T}}\underline{\mathbf{V}}^{-1}$  (B-58)

### Mobile Zone: Solution in Eigenvector Coordinate System

Selecting an arbitrary row from the matrix equation of (B-56), we have to solve:

$$v\underline{\mathbf{c}} + Aq\underline{\mathbf{c}}' - A(h^{-1}\underline{\boldsymbol{\delta}} + d)\underline{\mathbf{c}}'' = 0 \quad (\text{B-59})$$

Assume a general solution to Equation (B-59) of the form:

$$\underline{\mathbf{c}}(x) = a e^{bx} \quad (\text{B-60})$$

Substituting (B-60) into (B-59) gives:

$$a(v + Aqb - A(h^{-1}\underline{\boldsymbol{\delta}} + d)b^2)e^{bx} = 0 \quad (\text{B-61})$$

If  $a$  is non-zero,  $b$  must satisfy:

$$b^2 - \frac{q}{(h^{-1}\underline{\boldsymbol{\delta}} + d)}b - \frac{v}{A(h^{-1}\underline{\boldsymbol{\delta}} + d)} = 0 \quad (\text{B-62})$$

This has two possible solutions,

$$b = \frac{q}{2(h^{-1}\underline{\boldsymbol{\delta}} + d)} \left[ 1 \pm \sqrt{1 + \frac{4v(h^{-1}\underline{\boldsymbol{\delta}} + d)}{Aq^2}} \right] \quad (\text{B-63})$$

Note that the solutions for  $b$  are complex, because the eigenvalue  $v$  is complex.

### Mobile Zone: Boundary Conditions

It is assumed that  $\underline{\mathbf{c}}$  approaches zero as  $x$  approaches infinity. This will be the case provided there is a non-zero decay rate, or non-zero dispersivity, or some sort of storage zone exists. If none of these is the case, GoldSim will automatically add a very small dispersivity in order to stabilize the solution.

Note that the formula (B-63) for  $b$  implies that only one of the two possible solutions will have a negative real part. The other solution will be unbounded at  $x = \text{infinity}$ , and so the corresponding value for  $a$  in (B-60) must equal 0, and the

term can be ignored. Thus, one of the two roots for  $b$  will be the active one in every case.

Letting  $b$  be the root with  $\text{Re}(b) < 0$ , then since  $e^{b0}=1$ , using (B-54) we can express the known flux at  $x=0$  as:

$$\underline{f}_0 = aA(hq - (\delta + dh)b) \quad (\text{B-64})$$

Thus 
$$a = \frac{\underline{f}_0}{A(hq - (\delta + dh)b)} \quad (\text{B-65})$$

**Mobile Zone: Solution for Transfer Matrix**

Substituting the solution for  $a$  into (B-60) gives the solution for the concentration, in the transformed coordinates:

$$\underline{c} = \frac{\underline{f}_0}{A(hq - (\delta + dh)b)} e^{bx} \quad (\text{B-66})$$

and from (B-54) the flux is

$$\underline{f} = \frac{\underline{f}_0}{A(hq - (\delta + dh)b)} (A(hq - (\delta + dh)b)) e^{bx} = \underline{f}_0 e^{bx} \quad (\text{B-67})$$

Thus using (B-57):

$$\underline{\mathbf{T}} = [e^{bL}] \quad (\text{B-68})$$

For a source region distributed over a length  $S$  from the beginning of the Pipe, Equation (B-68) can be simply integrated to give:

$$\underline{\mathbf{T}} = \frac{[e^{bL} - e^{b(L-S)}]}{Sb} \quad (\text{B-68a})$$

So from (B-58) the desired transfer matrix for the Pipe pathway is simply:

$$\underline{\mathbf{T}} = \mathbf{V}[e^{bL}]\mathbf{V}^{-1} \quad (\text{B-69})$$

or, for a distributed source region,

$$\underline{\mathbf{T}} = \mathbf{V}\left[\frac{[e^{bL} - e^{b(L-S)}]}{Sb}\right]\mathbf{V}^{-1} \quad (\text{B-69a})$$

**Mathematical Representation of Matrix Diffusion Zones**

The equations for matrix diffusion are quite similar to those for the flowing zone. There is no advective flux, however, and the dispersive flux is replaced by a diffusive flux. The matrix block is assumed to have an effective thickness of  $t$ . For fracture systems  $t$  is typically half of the average fracture spacing, for porous medium flow it is the effective radius of the solid particles. The distance into the matrix block is defined by  $x$ , which ranges from 0 at the interface with the flowing zone to  $t$  at the inner boundary of the block.

For many fracture systems, the matrix block sizes will be variable. To represent this, the GoldSim implementation allows the user to specify a minimum and a maximum matrix-block thickness,  $t_{\min}$  and  $t_{\max}$ . GoldSim then simply integrates the kernel-functions for the block transfer matrices over the specified range of thicknesses, to represent a uniform distribution of the block thickness population (with respect to their area of intersection with the perimeter of the mobile zone).

Additionally, it is possible for different classes of matrix block to be connected to a specific fracture. For example, in a fault zone there may be both small internal blocks of centimeter to meter scale, and also the external rock matrix of much greater extent and probably different properties. GoldSim allows the user to define up to three separate classes of matrix block for a specific fracture, and allocate a specific fraction of the fracture's perimeter to each class.

To mathematically represent matrix diffusion, we solve for a transfer matrix  $\mathbf{X}$ , that converts the vector of concentrations in the flowing zone,  $\mathbf{c}_f$ , into a vector of mass flux rates from the flowing zone into the storage zone.

### **Matrix Diffusion Zones: Governing Equation**

The symbols used in this section are as follows:

$A$	=	cross-sectional area of the matrix, which may change with the distance into the matrix ( $L^2$ );
$A_0$	=	Area at the interface of the matrix with the mobile zone, based on allocating a fraction of the perimeter to each matrix diffusion zone ( $L^2$ );
$a_r$	=	coefficient used in the solution;
$b_r$	=	coefficient used in the solution;
$g$	=	Coefficient in formula for area, $A_0e^{gx}$
$\mathbf{c}$	=	vector of dissolved species concentrations in the matrix pores, with parents preceding daughters ( $M/L^3$ );
$\mathbf{c}'$	=	$\partial\mathbf{c}/\partial x$ , the first derivative of $\mathbf{c}$ with respect to distance $x$ ( $M/L^4$ );
$\mathbf{c}''$	=	$\partial^2\mathbf{c}/\partial x^2$ , the second derivative of $\mathbf{c}$ with respect to distance $x$ ( $M/L^5$ );
$e_r$	=	effective diffusivity of species $r$ , defined below in Equation B-70a ( $L^2/T$ );
$\mathbf{E}$	=	diagonal matrix of effective diffusivities ( $L^2/T$ );
$\mathbf{D}$	=	matrix of decay/ingrowth rate factors ( $T^{-1}$ );
$\mathbf{f}$	=	vector of mass fluxes in the $x$ direction ( $M/T$ );
$L$	=	pathway length ( $L$ );
$\mathbf{M}$	=	$[\mathbf{M}_{r \rightarrow c}]$ is a matrix used in the solution of the Laplace transformed equations
$\mathbf{N}_a$	=	diagonal matrix of available porosities for the porous medium in the matrix diffusion zone;
$\mathbf{R}$	=	diagonal matrix of the retardation factors in the matrix, defined below in Equation B-70b;
$t$	=	block thickness ( $L$ );
$t_{\min}$	=	minimum block thickness ( $L$ );
$t_{\max}$	=	maximum block thickness ( $L$ );
$\mathbf{T}$	=	matrix used in solution;
$s$	=	the (complex) Laplace variable;
$\mathbf{V}$	=	a matrix whose columns are the eigenvectors of $\mathbf{M}$ ;
$\mathbf{v}_r$	=	the $r$ 'th eigenvector of $\mathbf{M}$ ;

- $v_r$  = the  $r$ 'th eigenvalue of  $\mathbf{M}$ ;
- $x$  = the direction of diffusive transport, which is orthogonal to the mobile zone's  $x$ -direction; and
- $\mathbf{X}$  = transfer matrix for fluxes from the mobile zone to the storage zone (M/T).

The effective diffusivity term mentioned above is defined as follows:

$$e_r = n_r \tau d_{rw} \quad (\text{B-70a})$$

where  $n_r$  is the available porosity for species  $r$ ,  $\tau$  is the tortuosity of the matrix medium, and  $d_{rw}$  is the free water diffusivity of species  $r$ .

The retardation factor in the matrix is defined as follows:

$$R = (\rho K_s + n_s) / n_s \quad (\text{B-70b})$$

where  $\rho$  is the dry bulk density of the matrix material,  $K_s$  is the partition coefficient for species  $s$  for the matrix material ( $L^3/M$ ), and  $n_s$  is the available porosity of the matrix material for species  $s$ .

Consider an infinitesimal volume of the diffusive zone, of area  $A$  and length  $dx$ . The solute concentrations can be expressed as a function of distance along the zone,  $x$ . The amount of dissolved mass is  $dxAN_a\mathbf{c}$ , and the total amount of mass is  $dxAN_a\mathbf{R}\mathbf{c}$ . There are two processes which change the amount of mass: decay and diffusive transport. The rate of change (increase) of the total mass due to each process is as follows:

- *Decay.* The rate of change of the total mass due to decay is  $dxADN_a\mathbf{R}\mathbf{c}$ , where the  $\mathbf{D}$  is the matrix of decay and ingrowth coefficients.
- *Diffusive transport.* The diffusive flux in the  $x$  direction is  $-A\mathbf{E}\mathbf{c}'$ . The rate of change of the total mass due to diffusion equals  $dx$  times the derivative of the flux, or  $dx\{A\mathbf{E}\mathbf{c}'' + A'\mathbf{E}\mathbf{c}'\}$ .

The general differential equation for the conservation of mass in the diffusive zone is thus:

$$AN_a\mathbf{R} \frac{\partial \mathbf{c}}{\partial t} dx = AN_a\mathbf{D}\mathbf{R}\mathbf{c} dx + A\mathbf{E}\mathbf{c}'' dx + A'\mathbf{E}\mathbf{c}' dx \quad (\text{B-71})$$

or 
$$\mathbf{E}^{-1}\mathbf{N}_a\mathbf{R} \frac{\partial \mathbf{c}}{\partial t} = \mathbf{E}^{-1}\mathbf{N}_a\mathbf{D}\mathbf{R}\mathbf{c} + \mathbf{c}'' + \frac{A'}{A}\mathbf{c}' \quad (\text{B-72})$$

**Matrix Diffusion Zones:  
General Solution**

Taking the Laplace transform of Equation (B-72) simply results in replacing  $\mathbf{c}$  by  $\mathbf{c}^*$ , and replacing the time-derivative of  $\mathbf{c}$  by  $s\mathbf{c}^*$ :

$$\mathbf{M}\mathbf{c}^* - \frac{A'}{A}\mathbf{c}^{*'} - \mathbf{c}^{*''} = 0 \quad (\text{B-73})$$

where 
$$\mathbf{M} = \mathbf{E}^{-1}\mathbf{N}_a[\mathbf{I} - \mathbf{D}]\mathbf{R}$$

The transformed flux is:

$$\mathbf{f}^* = -A\mathbf{E}\mathbf{c}^{*'} \quad (\text{B-74})$$

**Matrix Diffusion Zones:  
Boundary Conditions**

There is no flux at  $x=t$ , which means that  $\mathbf{c}^{*'}(t)=0$ . At the interface with the mobile zone, the concentration equals that in the mobile zone, i.e.,  $\mathbf{c}^*(0)=\mathbf{c}_m^*$ .

**Matrix Diffusion Zones:  
Eigenvector Coordinate  
Transformation**

These boundary conditions convert directly to the eigenvector coordinate system described below.

Similarly to the solution for the flowing zone, define the transformed concentrations and fluxes as  $\underline{c}$  and  $\underline{f}$ , respectively. Let

$$\text{the concentration } \underline{c}^* = \mathbf{V}\underline{c}; \quad \underline{c} = \mathbf{V}^{-1}\underline{c}^* \quad (\text{B-75})$$

$$\text{and the flux } \underline{f}^* = \mathbf{V}\underline{f}; \quad \underline{f} = \mathbf{V}^{-1}\underline{f}^* \quad (\text{B-76})$$

$$\text{so from (B-74) } \underline{f} = -\mathbf{A}\mathbf{E}\underline{c} \quad (\text{B-77})$$

Substituting (B-75) into (B-73), and pre-multiplying by  $\mathbf{V}^{-1}$  gives:

$$\mathbf{V}^{-1}\mathbf{M}\mathbf{V}\underline{c} - \frac{\mathbf{A}'}{\mathbf{A}}\underline{c}' - \underline{c}'' = \mathbf{0} \quad (\text{B-78})$$

Recall that by the definition of the eigenvalues,  $\mathbf{M}\mathbf{V} = [\mathbf{v}_r]\mathbf{V}$ , so the preceding equation becomes:

$$[\mathbf{v}_r]\underline{c} - \frac{\mathbf{A}'}{\mathbf{A}}\underline{c}' - \underline{c}'' = \mathbf{0} \quad (\text{B-79})$$

The  $[\mathbf{v}_r]$  matrix of eigenvalues in Equation (B-79) is diagonal, so each row of (B-79) represents a separate ordinary differential equation. The following sections will develop the solution for an arbitrary member of this set of differential equations, for different geometries of the matrix-diffusion zone.

The solutions will lead to the eigenvector-transformed transfer matrix for the immobile zone,  $\underline{\mathbf{X}}$ , where:

$$\underline{f}(t) = \underline{\mathbf{X}}\underline{c}_m \quad (\text{B-80})$$

Substituting  $\mathbf{V}^{-1}\underline{f}^*$  for  $\underline{f}$  and pre-multiplying by  $\mathbf{V}$  gives the solution for the transfer matrix in the original coordinate system:

$$\underline{f}^*(t) = \mathbf{V}\underline{\mathbf{X}}\mathbf{V}^{-1}\underline{c}_m^* \quad (\text{B-81})$$

$$\text{i.e., the transfer matrix is } \underline{\mathbf{X}} = \mathbf{V}\underline{\mathbf{X}}\mathbf{V}^{-1} \quad (\text{B-82})$$

**Matrix Diffusion: Slab  
Blocks**

For slab-type matrix blocks with constant area A, row r from (B-79) becomes:

$$v_r \underline{c} - \underline{c}'' = 0 \quad (\text{B-83})$$

The solution to this equation is:

$$\underline{c} = \left( \cosh(\sqrt{v_r} x) - \tanh(\sqrt{v_r} t) \sinh(\sqrt{v_r} x) \right) \underline{c}_m \quad (\text{B-84})$$

From (B-77) the transformed flux at the interface with the mobile zone is:

$$\underline{f}(0) = -A_0 e_r \sqrt{v_r} \tanh(\sqrt{v_r} t) \underline{c}_m \quad (\text{B-85})$$

where  $e_r$  is the effective diffusivity for the r'th species.

Finally, from (B-82) the transfer matrix for the slab is:

$$\underline{\mathbf{X}} = \mathbf{V} \left[ -A_0 e_r \sqrt{v_r} \tanh(\sqrt{v_r} t) \right] \mathbf{V}^{-1} \quad (\text{B-86})$$

**Matrix Diffusion:  
Spherical Blocks**

For spherical matrix blocks of radius  $t$ ,  $A=A_0(1-x/t)^2$ , and  $A'/A=-2/(t-x)$ . Row  $r$  from (B-79) becomes:

$$v_r \underline{c} + \left( \frac{2}{t-x} \right) \underline{c}' - \underline{c}'' = 0 \quad (\text{B-87})$$

The solution to this equation is (Barker, 1985):

$$\underline{c} = \frac{t \sinh(\sqrt{v_r}(t-x))}{(t-x) \sinh(\sqrt{v_r}t)} \underline{c}_m \quad (\text{B-88})$$

The first derivative of  $\underline{c}$  is:

$$\underline{c}' = \left[ -\frac{t\sqrt{v_r} \cosh(\sqrt{v_r}(t-x))}{(t-x) \sinh(\sqrt{v_r}t)} + \frac{t \sinh(\sqrt{v_r}(t-x))}{(t-x)^2 \sinh(\sqrt{v_r}t)} \right] \underline{c}_m$$

(B-89)

From (B-77) the transformed flux at the interface with the mobile zone ( $x=0$ ) is:

$$\underline{f}(0) = -A_0 e_r \left[ \frac{t\sqrt{v_r} \cosh(\sqrt{v_r}t)}{t \sinh(\sqrt{v_r}t)} - \frac{t \sinh(\sqrt{v_r}t)}{t^2 \sinh(\sqrt{v_r}t)} \right] \underline{c}_m \quad (\text{B-90})$$

$$\underline{f}(0) = A_0 e_r \left[ \frac{1}{t} - \frac{\sqrt{v_r}}{\tanh(\sqrt{v_r}t)} \right] \underline{c}_m \quad (\text{B-91})$$

So, from (B-82) the transfer matrix for the sphere is:

$$\mathbf{X} = \mathbf{V} \left[ A_0 e_r \left[ \frac{1}{t} - \frac{\sqrt{v_r}}{\tanh(\sqrt{v_r}t)} \right] \right] \mathbf{V}^{-1} \quad (\text{B-92})$$

**Matrix Diffusion:  
Exponential-Area  
Blocks**

GoldSim also provides a third geometric form for matrix blocks, which may be used to approximate the solution to a ribbon-like ‘slot’ pathway where the area of the matrix block increases with the distance away from the fracture. The solution presented below is for an area  $A(x) = A_0 e^{gx}$  which increases exponentially up to the maximum diffusion depth  $d$ . GoldSim uses a  $g$ -value of 2 for its solution of this problem.

Assume a general solution of row  $r$  of (B-79) of the form:

$$\underline{c} = a e^{bx} \quad (\text{B-93})$$

Substituting into (B-79) gives:

$$a v_r e^{bx} - \frac{A'}{A} a b e^{bx} - a b^2 e^{bx} = 0$$

or 
$$a \left[ v_r - \frac{A'}{A} b - b^2 \right] e^{bx} = 0 \quad (\text{B-94})$$

For this equation to be satisfied for all  $y$  values between 0 and  $t$ ,  $A'/A$  must be a constant ratio, so that  $A = A_0 e^{gx}$ , i.e.,  $A'/A = g$ . Note that the slab solution represents a special case of this with  $g=0$ .

If  $a$  is non-zero,  $b$  must satisfy:

$$b^2 + gb - v_r = 0 \quad (\text{B-95})$$

Thus  $b$  has two possible solutions,

$$b^{+-} = \frac{-g}{2} \pm \sqrt{\left(\frac{g}{2}\right)^2 + v_r} \quad (\text{B-96})$$

In general, either solution is valid. We will refer to the two  $b$  values as  $b^+$  and  $b^-$ , and to their corresponding  $a$  values as  $a^+$  and  $a^-$ . We can then rewrite (B-93) as:

$$\underline{c} = a^+ e^{b^+x} + a^- e^{b^-x} \quad (\text{B-97})$$

Note that the  $b^{+-}$  values are complex, because  $v_r$  is complex.

Because the flux at  $x=t$  equals zero,  $c'(t) = 0$ .

Differentiating (B-97) and equating to zero gives:

$$a^+ b^+ e^{b^+t} + a^- b^- e^{b^-t} = 0 \quad (\text{B-98})$$

$$\text{so } a^+ = -a^- \frac{b^-}{b^+} \frac{e^{b^-t}}{e^{b^+t}} \quad (\text{B-99})$$

$$\text{or } a^+ + a^- = a^- \left[ 1 - \frac{b^-}{b^+} e^{(b^- - b^+)t} \right] \quad (\text{B-100})$$

Setting the transformed concentrations at  $x=0$  equal to the mobile-zone concentration vector,  $\underline{c}_m$  results in the following:

$$a_r^+ + a_r^- = \underline{c}_m \quad (\text{B-101})$$

In order to solve for the flux at  $x=0$ , we will need to evaluate the term  $(a^+ b^+ + a^- b^-)$ .

From (B-100):

$$a^- \left[ 1 - \frac{b^-}{b^+} e^{(b^- - b^+)t} \right] = \underline{c}_m \quad (\text{B-102})$$

And using (B-99):

$$a^+ = \frac{-b^- e^{(b^- - b^+)t}}{b^+ - b^- e^{(b^- - b^+)t}} \underline{c}_m^* \quad (\text{B-103})$$

Therefore,

$$\{a^+ b^+ + a^- b^-\} = \left[ \frac{-b^+ b^- e^{(b^- - b^+)t}}{b^+ - b^- e^{(b^- - b^+)t}} + \frac{b^+ b^-}{b^+ - b^- e^{(b^- - b^+)t}} \right] \underline{c}_m \quad (\text{B-104})$$

$$\text{and } \{a^+ b^+ + a^- b^-\} = \left[ \frac{b^+ b^- (1 - e^{(b^- - b^+)t})}{b^+ - b^- e^{(b^- - b^+)t}} \right] \underline{c}_m \quad (\text{B-105})$$

From (B-77) and (B-97) the transformed flux at  $x=0$  is:

$$\underline{f}(0) = -A_o e_r \{a^+ b^+ + a^- b^-\} \quad (\text{B-106})$$

Using (B-82) the desired transfer matrix is therefore:

$$\mathbf{X} = \mathbf{V} \left[ \frac{-A_o e_r b^+ b^- (1 - e^{(b^- - b^+)t})}{b^+ - b^- e^{(b^- - b^+)t}} \right] \mathbf{V}^{-1} \quad (\text{B-107})$$

Note that for the slab-diffusion case where  $g=0$ , (B-107) is equivalent to (B-86).

For positive  $s$  values, the real part of  $(b^- - b^+)$  is always negative, so in the limit of large matrix thicknesses,  $\mathbf{X}$  simplifies to:

$$\mathbf{X} = \mathbf{V} \left\{ -A_o e_r b_r^- \right\} \mathbf{V}^{-1} \quad (\text{B-108})$$

### Matrix Diffusion: Skin Zone

For fracture flow systems, it may be the case that the matrix rock adjacent to the flowing fractures has different properties than the rock further from the fracture. This local “alteration zone” may be due to geochemical or geothermal effects, and frequently results in increased porosity and sorptivity of the alteration zone.

The GoldSim Pipe pathway allows the user to specify such a “skin” zone. Diffusion through the skin material is assumed to be uniform (i.e., slab-diffusion). Thus, the solution for the skin zone is similar to that for the slab matrix blocks, except that at the end of the skin zone the boundary condition is not  $c'=0$ . Instead the boundary condition consists of a concentration-flux relationship specified by the transfer matrix for the outer region of the matrix.

In principle, it is possible to define a series of skin layers using the same approach, as shown by Barten (1996). However, the GoldSim implementation only provides for a single skin layer.

Because of the more complex boundary condition, it is not possible to fully decouple the individual differential equation for each eigenvector. Thus, the following derivation addresses the full matrix equations. However, the eigenvector transformation is still used in order to diagonalize all but the boundary condition at  $x=t$ .

Assume a solution for the transformed concentrations of the form:

$$\underline{c} = \{c_r\} = \{a_r \sinh(\sqrt{v_r} x) + b_r \cosh(\sqrt{v_r} x)\} \quad (\text{B-109})$$

From (B-77), the transformed flux is:

$$\underline{f} = -\mathbf{A}\mathbf{E}\underline{c}' = \left\{ \mathbf{A}e_r c_r' \right\} = \left\{ \mathbf{A}e_r \sqrt{v_r} (a_r \cosh(\sqrt{v_r} x) + b_r \sinh(\sqrt{v_r} x)) \right\} \quad (\text{B-110})$$

The concentration at  $x=0$  equals that in the mobile zone, so:

$$\underline{c}(0) = \{b_r\} = \underline{c}_m = \{c_{mr}\} \quad (\text{B-111})$$

At  $x=t$ , the end of the skin, assume a transfer matrix  $\mathbf{X}_a$  represents the additional matrix diffusion zone(s). This can be transformed to the eigenvector coordinate system as follows:

$$\underline{f}^*(t) = \mathbf{X}_a \underline{c}^*(t) \quad (\text{B-112})$$

or, replacing  $\underline{c}^*$  by  $\mathbf{V}\underline{c}$  and pre-multiplying by  $\mathbf{V}^{-1}$ :

$$\underline{f}(t) = \mathbf{V}^{-1} \mathbf{X}_a \mathbf{V} \underline{c}(t) = \mathbf{T}_a \underline{c}(t) \quad (\text{B-113})$$

Where  $\mathbf{T}_a$  represents the  $\mathbf{X}_a$  matrix transformed to the eigenvector coordinates.

Substituting (B-109) and (B-110) into (B-113), and collecting terms in  $a_r$  and  $c_{mr}$  leads to:

$$-\mathbf{T}_a \{a_r t_r\} - \{Ae_r a_r \sqrt{v_r}\} = \mathbf{T}_a \{c_{mr}\} + \{Ae_r c_{mr} t_r \sqrt{v_r}\} \quad (\text{B-114})$$

where

$$t_r = \tanh(\sqrt{v_r} t) \quad (\text{B-115})$$

The transformed flux from the flowing zone is:

$$\underline{\mathbf{f}}(0) = \{Ae_r \sqrt{v_r} a_r\} \quad (\text{B-116})$$

After manipulation of (B-114), we get:

$$\underline{\mathbf{f}}(0) = \{Ae_r a_r \sqrt{v_r}\} = \left[ -\mathbf{T}_a \left[ \frac{t_r}{Ae_r} \right] - 1 \right]^{-1} \left[ \mathbf{T}_a \left[ \sqrt{v_r} \right] + \{Ae_r t_r \sqrt{v_r}\} \right] \{c_{mr}\} \quad (\text{B-117})$$

Finally, from (B-82) the transfer matrix for the skin-enhanced matrix zone is:

$$\mathbf{X} = \mathbf{V} \left[ -\mathbf{T}_a \left[ \frac{t_r}{Ae_r} \right] - 1 \right]^{-1} \left[ \mathbf{T}_a \left[ \sqrt{v_r} \right] + \{Ae_r t_r \sqrt{v_r}\} \right] \mathbf{V}^{-1} \quad (\text{B-118})$$

### **Mathematical Representation of Stagnant Dispersive Zone**

GoldSim's conceptual model of dispersive storage zones assumes that some fraction  $f_{im}$  of the primary Pipe pathway is in fact stagnant. However, there is a continual exchange of water between the mobile zone and the stagnant zone. The rate of exchange is defined by an advective mixing parameter,  $\beta$  which represents the probability of an individual species molecule moving from the flowing to the stagnant zone, per meter of distance traveled along the flowing zone.

If  $\beta L / f_{im}$  is much larger than 1, the two zones are well mixed and the pathway behaves as if the stagnant zone was combined with the flowing zone, with a reduced velocity based on the total porosity as a result.

If  $\beta L / f_{im}$  is somewhat larger than 1, the zones are partially mixed and the pathway will show dispersion. As  $\beta L / f_{im}$  reduces towards 1, the pathway breakthrough curve becomes asymmetrical, with a sharp rise and an elongated tail. At the lower values of  $\beta L / f_{im}$ , the breakthrough is characterized by a spike of undispersed solute, followed by an elongated tail due to release from the stagnant zone back to the mobile zone.

To mathematically represent the stagnant dispersive zone, we solve for a transfer matrix  $\mathbf{X}$ , that converts the vector of concentrations in the mobile zone,  $\mathbf{c}_r$ , into a vector of mass flux rates from the mobile zone into the storage zone.

### **Stagnant Dispersive Zone: Governing Equation**

The following symbols are used in this section:

$\beta$	probability of an individual solute molecule moving from the flowing to the stagnant zone, per unit distance traveled along the flowing zone ( $L^{-1}$ );
$\mathbf{c}_m$	vector of dissolved species concentrations in the mobile pores ( $M/L^3$ );

$\mathbf{c}_{im}$	vector of dissolved species concentrations in the stagnant pores ( $M/L^3$ );
$\mathbf{D}$	matrix of decay/ingrowth rate factors ( $T^{-1}$ );
$f_{im}$	fraction of the pathway pores that are stagnant;
$\mathbf{f}_{m-im}$	transformed mass flux from mobile to stagnant pores;
$\mathbf{M}$	a matrix used in the solution of the Laplace transformed equations;
$\mathbf{N}_a$	Diagonal matrix of available porosities for the porous medium in the stagnant zone;
$\mathbf{R}$	Diagonal matrix of the retardation factors in the stagnant zone (see Equation B-30 for definition of individual items); and
$\mathbf{X}$	transfer matrix for fluxes from the flowing zone to the storage zone ( $M/T$ ).

The total amount of solute in the stagnant pores, per unit length of the pathway, is  $f_{im} \mathbf{A} \mathbf{N}_a \mathbf{R} \mathbf{c}_{im}$ , and its rate of change due to decay is  $f_{im} \mathbf{A} \mathbf{N}_a \mathbf{D} \mathbf{R} \mathbf{c}_{im}$ .

The flow between the mobile and stagnant zones is  $\beta A q$  per unit length of the pathway, so the rate of transfer of species from the mobile to the stagnant zone is  $f_{im} \beta A q (\mathbf{c}_m - \mathbf{c}_{im})$

The equation for the conservation of mass in a unit length of the stagnant zone is thus:

$$f_{im} \mathbf{A} \mathbf{N}_a \mathbf{R} \frac{\partial \mathbf{c}_{im}}{\partial t} = f_{im} \mathbf{A} \mathbf{N}_a \mathbf{D} \mathbf{R} \mathbf{c}_{im} + \beta A q (\mathbf{c}_m - \mathbf{c}_{im}) \quad (\text{B-119})$$

**Stagnant Dispersive Zone: Derivation of the Transfer Matrix**

Taking the Laplace transform of Equation (B-119) gives

$$\mathbf{M} \mathbf{c}_{im}^* = \beta A q (\mathbf{c}_m^* - \mathbf{c}_{im}^*) \quad (\text{B-120})$$

where  $\mathbf{M} = f_{im} \mathbf{A} n [s \mathbf{I} - \mathbf{D}] \mathbf{R}$  (B-121)

so  $[\beta A q \mathbf{I} + \mathbf{M}] \mathbf{c}_{im}^* = \beta A q \mathbf{c}_m^*$  (B-122)

or  $\mathbf{c}_{im}^* = [\beta A q \mathbf{I} + \mathbf{M}]^{-1} \beta A q \mathbf{c}_m^*$  (B-123)

The transformed flux from the mobile to the stagnant zone is

$$\begin{aligned} \mathbf{f}_{m-im} &= \beta A q (\mathbf{c}_m^* - \mathbf{c}_{im}^*) \\ \mathbf{f}_{m-im} &= \beta A q \left\{ \mathbf{I} - \beta A q [\beta A q \mathbf{I} + \mathbf{M}]^{-1} \right\} \mathbf{c}_m^* \end{aligned} \quad (\text{B-124})$$

After simplification, this gives

$$\mathbf{f}_{m-im} = \beta A q \mathbf{M} [\beta A q \mathbf{I} + \mathbf{M}]^{-1} \mathbf{c}_m^* \quad (\text{B-125})$$

This defines the transfer matrix,  $\mathbf{X}$ , for mass transfer from mobile to stagnant pores, as used in Equation B-48.

## Plume Function Details

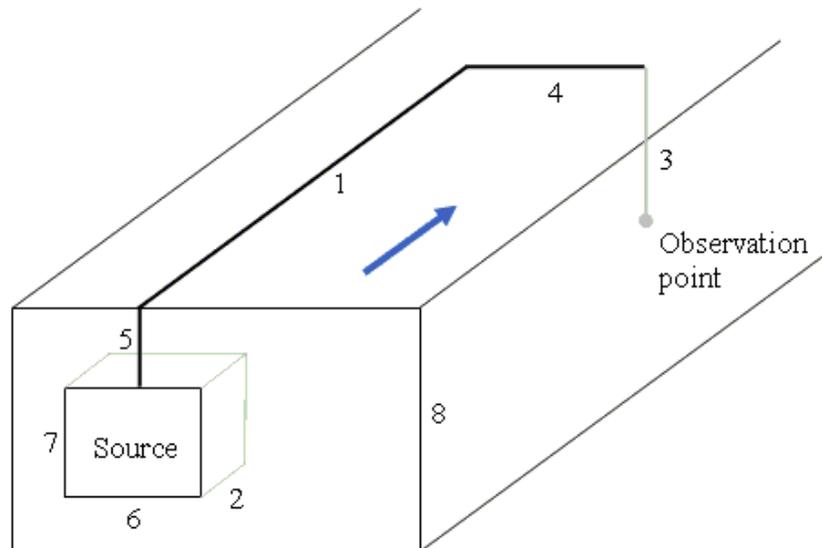
Since Aquifers and Pipes are meant to represent one-dimensional conduits, the concentration reported by these two pathways represents the average concentration discharging from the pathway, and any spatial variation in the concentration (perpendicular to the flow direction) is not represented.

In many cases, however, real world concentrations will vary spatially at the end of a flow path due to dispersion in the horizontal or vertical transverse direction and/or a source term which is not uniformly distributed across the area of the conduit being simulated.

In order to allow you to address this spatial variation, GoldSim provides a special function which returns a correction factor which can be used to multiply the Aquifer's or Pipe's concentration output in order to compute the actual (as opposed to spatially-averaged) concentration at an observation point at some distance perpendicular to the flow path at the end of the pathway.

The *Plume function* (which is analogous to other GoldSim functions like *sin* or *max*) has eleven input arguments which describe the properties of the pathway to which you wish to apply the correction, the size of the source, the dispersive properties of the pathway, and the exact location of the observation point. The source is assumed to be a point, rectangle or box centered on the midpoint of the flow path (the pathway), and the observation point is located at the end of the pathway some specified distance from the centerline.

The following diagram illustrates the various input arguments required by the Plume function.



The arguments are as follows (the numbers reference lengths in the figure above):

$X_L$	length of Pathway (and the longitudinal position of the observation point) [1]
$A$	cross-sectional area of the Pathway
$L_s$	length of the source parallel to the flow direction [2]
$X_V$	vertical position of the observation point [3]

$X_T$	transverse position of the observation point [4]
$D_s$	vertical depth to the top of the source from the top of the aquifer [5]
$W_s$	width of the source, transverse to the aquifer flow [6]
$b_s$	thickness of the source [7]
$b$	thickness of the aquifer [8]
$\alpha_T$	dispersivity in the transverse (horizontal) direction
$\alpha_V$	dispersivity in the vertical direction

All of these arguments with the exception of  $A$  have dimensions of Length.  $A$  has dimension of Length<sup>2</sup>. It is critical that  $X_L$  and  $A$  are the same values assigned to the Pathway itself.

The manner in which GoldSim uses these values to compute the correction factor (referred to in the discussion below as *dilute*) is described below (thanks to John Tauxe of Neptune and Company for assisting in documenting these equations).

Note that *dilute* will always have a value greater than or equal to 0. It may be greater than 1 (as the concentration at a particular point, of course, may be greater than the average concentration).

## Calculating the Correction Factor

The value of *dilute* is calculated in parts, with all parts multiplied in the end:

$$dilute = dilute_{init} \times dilute_T \times dilute_V \tag{B-126}$$

Note that in some cases, one or more of these terms may be equal to unity, in effect removing its influence, or zero, in effect making the entire calculation equal to zero.

Initially, we  $dilute_{init}$  is set to the cross-sectional area of the Pathway,  $A$ . As the value of *dilute* is modified for dispersion effects in the subsequent calculations, it is twice divided by a length, leaving it dimensionless.

So far, we have:

$$dilute_{init} = A \tag{B-127}$$

## Relative Length Adjustment

The length  $X_L$  of the Pathway is assumed to be measured from the upstream end of the source. It is then modified in order to center the source at the longitudinal “origin.” The following cases are considered:

Case 1: if  $X_L \leq 0$ , then the point of observation is upstream of the source, and

$$dilute_{init} = 0 \tag{B-128}$$

At this point,  $X_L$  is also set to  $X_L = 1$  (with units of m implied), to preclude divide-by-zero errors.

Case 2: if  $X_L > L_s$ , then the point of observation is downstream of the source, and  $X_L$  is adjusted thus

$$X_L^* = X_L - \frac{L_s}{2} \quad (\text{B-129})$$

so that the “source” end of the Pathway is moved to the center of the source. This adjusted length is denoted  $X_L^*$ .

Case 3: if neither of the above cases is true, then  $X_L < L_s$ , meaning that the Pipe is shorter than the source. In this case,  $X_L$  is halved:

$$X_L^* = \frac{X_L}{2}. \quad (\text{B-130})$$

This, in effect, truncates the source to be the length of the Pathway, and the upstream end is moved to the center of the source. In the latter two cases, the value of  $dilute_{init}$  remains equal to  $A$ .

## Transverse Dispersion

To account for transverse (horizontal) dispersion, various cases are considered: a narrow (point) source, a wide source, and the case where the observation point is too far afield to be considered part of the plume.

### Narrow (Point) Source

A narrow source triggers the point-source solution for transverse dispersion. In comparing the source width  $W_s$  to the transverse standard deviation of the plume,  $\sqrt{2 \alpha_T X_L^*}$ , a narrow source solution is used if

$$W_s < \frac{\sqrt{2 \alpha_T X_L^*}}{100} \quad (\text{B-131})$$

In this case, the point-source solution is used, and the transverse portion of  $dilute$ , hereafter called  $dilute_T$ , assumes the form of the normal distribution density function:

$$dilute_T = \frac{\exp\left[-\frac{\left(\frac{X_T}{\sqrt{2 \alpha_T X_L^*}}\right)^2}{2}\right]}{\sqrt{2\pi}\sqrt{2 \alpha_T X_L^*}} = \frac{\exp\left(-\frac{X_T^2}{4 \alpha_T X_L^*}\right)}{\sqrt{4 \pi \alpha_T X_L^*}}. \quad (\text{B-132})$$

Recall that  $dilute_T$  is to be multiplied by  $dilute_{init}$  in order to arrive at the final correction factor.

### Wide (General) Source

A “wide” source, the general full solution, is indicated if the following is true:

$$W_s < 1,000,000 \times \sqrt{2 \alpha_T X_L^*}. \quad (\text{B-133})$$

This applies in the case where a source is not negligibly wide, and dispersion cannot be ignored. In this case, the point-source solution is integrated over the width of the source, and  $dilute_T$  is

$$dilute_T = \frac{\operatorname{erf}\left(\frac{X_T + \frac{W_s}{2}}{\sqrt{4 \alpha_T X_L^*}}\right) - \operatorname{erf}\left(\frac{X_T - \frac{W_s}{2}}{\sqrt{4 \alpha_T X_L^*}}\right)}{2 W_s}. \quad (\text{B-134})$$

### Negligible Transverse Dispersion

If neither of the previous two situations occurs, then the transverse dispersion is negligible (i.e., the plume does not spread at all), and the observation point is tested to see if it is inside or outside of the plume. The test for being outside the

plume is if the transverse location of the observation point is greater than half the source width from the plume centerline:

$$|X_T| > \frac{W_s}{2}. \quad (\text{B-135})$$

In effect, if the observation location is further from the centerline than the edge of the source, then it is out of the plume. If equation (B-135) holds true, then the point is outside the plume, and *dilute<sub>T</sub>* (and therefore *dilute*) is set to zero. Otherwise *dilute<sub>T</sub>* is set equal to the inverse of the source width, *W<sub>s</sub>*.

## Vertical Dispersion

In the case of dispersion in the vertical direction, again perpendicular to flow, five cases are considered: a fully mixed aquifer, a thin source, a thick source, no source geometry adjustment, and the case where the observation point is too shallow or deep to be considered part of the plume. Since the flow field is assumed to have natural boundaries on the top and bottom, but not on the sides, the calculation of concentrations at vertical locations within the aquifer takes advantage of superposed image source mathematics. Note that, unlike the transverse case, where the source is always centered horizontally, the vertical position of the source may be anywhere within the flow field. Similar to the transverse case, the vertical aspect of the source may be relatively thin or thick compared to vertical dispersion.

### Fully Mixed Aquifer

If an aquifer (or, more generically, the flow field) is sufficiently thin in comparison to dispersion in the vertical direction, then the flow field can be assumed to be fully mixed in the vertical direction, and no image sources are used. That is, if we compare the aquifer thickness *b* to the vertical standard deviation of the plume  $\sqrt{2 \alpha_V X_L^*}$ , and

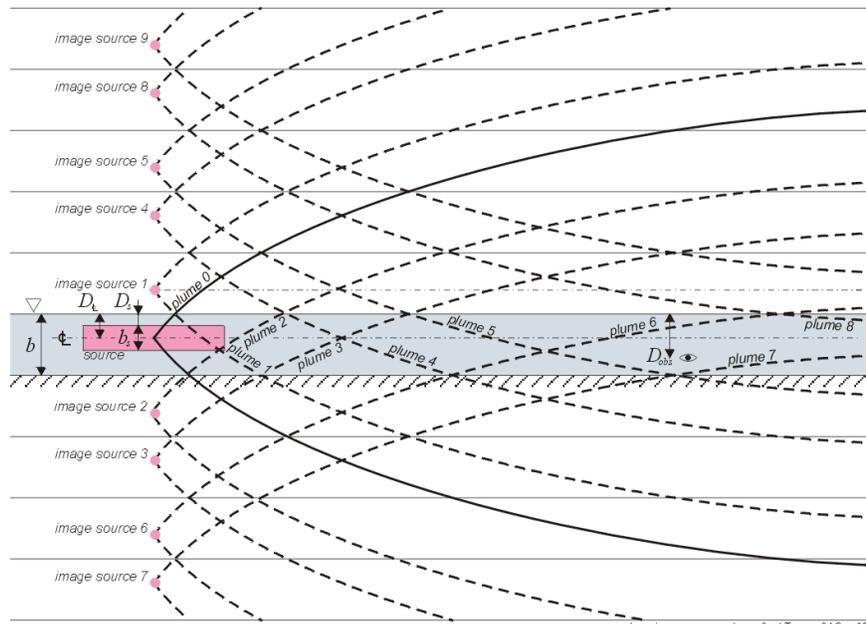
$$b < \frac{\sqrt{2 \alpha_V X_L^*}}{3} \quad (\text{B-136})$$

then *dilute* is merely divided by that thickness, so that the vertical term *dilute<sub>v</sub>* becomes

$$dilute_v = \frac{1}{b}. \quad (\text{B-137})$$

### Use of Image Sources to Represent Interaction with Top and/or Bottom of Aquifer

If the aquifer is not sufficiently thin to be considered fully mixed, it is examined for suitability in using nine image sources to refine the vertical distribution of contaminants, as illustrated in the figure below.



In effect, the plume from each image source, identical to the original source, is offset and its contribution to the concentrations in the aquifer is superimposed. This has the same effect as “bouncing” the original plume off the top and bottom of the aquifer.

Image sources are invoked if equation (B-136) is not satisfied, and analogous to equation (B-133),

$$b < 1,000,000 \times \sqrt{2 \alpha_V X_L^*} \tag{B-138}$$

If this inequality is not true, then no image sources are used, and no further changes are made to *dilute* for vertical dispersion (and the following sections testing for a thin or thick source are also precluded).

Use of Images for a Thin Source

A thin source triggers the point-source solution for vertical dispersion, expanded to include the additional image sources (the development of which is not covered here). In comparing the aquifer thickness *b* to the vertical standard deviation of the plume  $\sqrt{2 \alpha_V X_L^*}$ , a thin source solution is used if

$$b < \frac{\sqrt{2 \alpha_V X_L^*}}{100} \tag{B-139}$$

In this case, the point-source solution is used with *i* images at vertical locations  $X_{Vi}$  relative to the source’s vertical centerline, and *dilute*<sub>v</sub> is the summation of a number of normal distribution density terms:

$$dilate_v = \frac{\sum_i \exp\left(-\frac{X_{Vi}^2}{4 \alpha_V X_L^*}\right)}{\sqrt{4 \pi \alpha_V X_L^*}} \tag{B-140}$$

Note that *dilute*<sub>v</sub> is to be multiplied by *dilute*<sub>init</sub> and *dilute*<sub>T</sub> in order to arrive at the final correction factor.

If the criterion for using images is met, that is, equation (B-138) is true, and that for a thin source is not met, that is, equation (B-139) is false, then the source is assumed to be relatively thick.

Use of Images for a Thick Source

In the case of a source that is relatively thick in comparison to vertical dispersion, the point-source solution is integrated over the thickness of the source  $b_s$  and is summed over  $i$  image sources, so that  $dilute_V$  is

$$dilute_V = \frac{\sum_i \left[ \operatorname{erf} \left( \frac{X_{V_i} + \frac{b_s}{2}}{\sqrt{4 \alpha_V X_L^*}} \right) - \operatorname{erf} \left( \frac{X_{V_i} - \frac{b_s}{2}}{\sqrt{4 \alpha_V X_L^*}} \right) \right]}{2 b_s} \tag{B-141}$$

**Negligible Vertical Dispersion**

In the case where we still do not assume vertical mixing and also do not invoke the use of image sources, then a final test is made to determine whether the observation point is vertically outside the plume. If the vertical location of the observation point relative to the vertical centerline of the source is greater than half the source thickness, expressed as

$$|X_V| > \frac{b_s}{2} \tag{B-142}$$

then the observation point is considered to be out of the plume and  $dilute_V$  (and therefore  $dilute$ ) is set to zero. Otherwise  $dilute_V$  is set equal to the inverse of the source thickness.

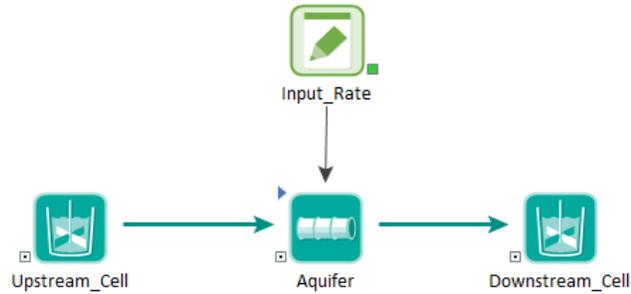
## Aquifer Pathway Details

An Aquifer pathway performs its computations by creating a temporary set of linked Cell elements during the simulation (while in Run Mode), which are subsequently removed at the end of the simulation. However, while in Run Mode, the pathways exist (and if you pause the model, can actually be viewed).

To illustrate this, and to explain how the various inputs for an Aquifer are mapped onto and treated within the temporary Cell network, we will consider a simple example. In this example, an Aquifer has been defined. Its key properties are as follows:

- The Number of Cells used to discretize the pathway is equal to five.
- The Aquifer contains an Infill Medium (Sand).
- The Aquifer has a single outflow (Q) to a downstream Cell.

While in Run Mode, an Aquifer pathway takes on some characteristics of a Container so that the temporary Cells can be viewed. In this example, if we pause the model during the simulation, the Aquifer pathway will look like this (i.e., like a Container, it has a small triangle in the upper left-hand corner of the element indicating that you can “look inside”):



If we click on the triangle to “look inside” the Aquifer, we see the following:



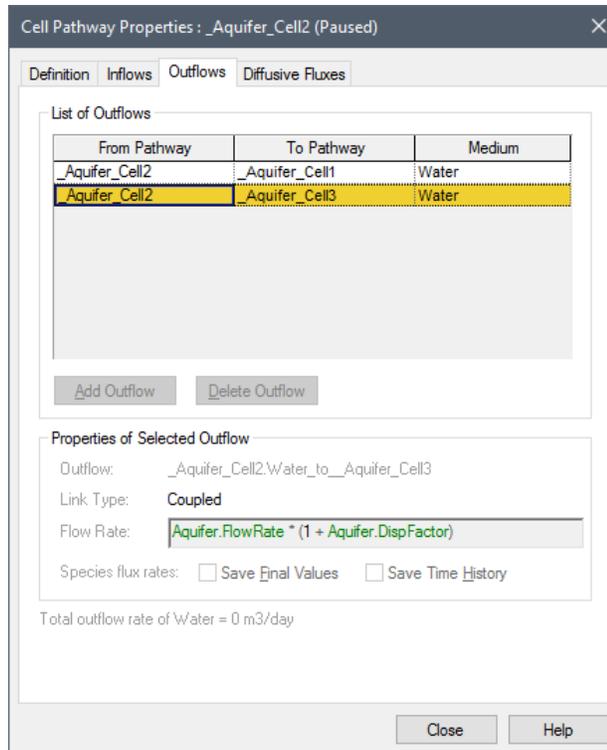
As can be seen, five temporary Cells have been created (named “\_pathwayname\_Celln”). Opening the first Cell, we can see how the Media are defined:

Medium	Amount	F	H	S
Water	$Aquifer.OtherCell.Length * Aquifer.Area * Sa$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Sand	$Aquifer.OtherCell.Length * Aquifer.Area * Sa$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

The media quantities are automatically computed based on the Aquifer properties (e.g., Length, Area, Saturation, Number of Cells) and media properties (density, porosity).

In effect, GoldSim has discretized the system into these five finite volumes.

To simulate advection and dispersion/diffusion through the linked Cells, GoldSim automatically creates a number of advective and diffusive flux links. For example, here is the Outflows tab from the second Cell:



There is an Outflow from Cell2 to Cell3. Note, however, that the Flow Rate that was specified when defining the element has been adjusted. The Flow Rate (downstream) from Cell2 to Cell3 is now defined as  $Q \cdot (1 + \text{DispFactor})$ , where

$$\text{DispFactor} = (n \alpha / L) - 0.5 \quad (\text{B-143})$$

In this equation,  $\alpha$  is the species dispersivity (dimensions of L), L is the pathway length (dimensions of L), and n is the number of cells.

Note that there is another Outflow in the Outflows tab, and it is from Cell2 to Cell1 (upstream!). If we were to look at this, we would see that this upstream Flow Rate was defined as  $Q \cdot \text{DispFactor}$ . That is, in addition to the downstream flow that we would expect (Q), GoldSim has added two “fictitious” flows equal to  $Q \cdot \text{DispFactor}$  (one upstream and one downstream). Note that since one fictitious flow is downgradient and one is upgradient, the net of these two flows is zero. However, they have the effect of representing longitudinal dispersion in the pathway.

In effect, what GoldSim is doing is using the Cells (the finite volumes) to solve the governing equation describing one-dimensional advective/dispersive transport.

To see how this is done, consider the governing differential equation for one dimensional advection/dispersion:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (\text{B-144})$$

where C is the concentration ( $M/L^3$ ), v is the seepage velocity ( $L/T$ ), D is the mechanical dispersion coefficient ( $L^2/T$ ), and x is the distance along the pathway (L). The first term represents dispersion, while the second represents advection.

We can approximate this equation using an implicit, centrally weighted finite difference scheme as follows:

$$\frac{C_j^{k+1} - C_j^k}{\Delta t} = \frac{D}{(\Delta x)^2} (C_{j+1}^{k+1} - 2C_j^{k+1} + C_{j-1}^{k+1}) - \frac{v}{\Delta x} (0.5C_{j+1}^{k+1} - 0.5C_{j-1}^{k+1}) \quad (\text{B-145})$$

In this equation,  $j$  is the current Cell,  $j-1$  is the upstream Cell and  $j+1$  is the downstream Cell.  $\Delta x$  is the effective length of each Cell,  $\Delta t$  is the timestep,  $k$  represents the current timestep and  $k+1$  represents the subsequent timestep.

We can rewrite this equation in terms of the mass rate of change by noting the following:

$$C_j = \frac{M_j}{\Delta x A \theta} \quad (\text{B-146})$$

where  $M_j$  is the mass in Cell  $j$ ,  $A$  is the cross-sectional area of the pathway ( $L^2$ ), and  $\theta$  is the porosity.

Equation (B-145) can then be written as follows:

$$\frac{M_j^{k+1} - M_j^k}{\Delta t} = \frac{A \theta D}{\Delta x} (C_{j+1}^{k+1} - 2C_j^{k+1} + C_{j-1}^{k+1}) - v A \theta (0.5C_{j+1}^{k+1} - 0.5C_{j-1}^{k+1}) \quad (\text{B-147})$$

The seepage velocity,  $v$  ( $L/T$ ), can be expressed in terms of the flow rate  $Q$  ( $L^3/T$ ), the cross-sectional area  $A$  ( $L^2$ ) and the porosity  $\theta$ :

$$v = \frac{Q}{\theta A} \quad (\text{B-148})$$

The mechanical dispersion coefficient  $D$  ( $L^2/T$ ) can be expressed in terms of the dispersivity  $\alpha$  ( $L$ ) and the seepage velocity:

$$D = \alpha v = \frac{\alpha Q}{\theta A} \quad (\text{B-149})$$

$\Delta x$  can be expressed in terms of the total pathway length  $L$  and the number of Cells  $n$ :

$$\Delta x = \frac{L}{n} \quad (\text{B-150})$$

Combining equations (B-148), (B-149) and (B-150) into (B-147) yields the following:

$$\frac{M_j^{k+1} - M_j^k}{\Delta t} = \frac{Q \alpha n}{L} (C_{j+1}^{k+1} - 2C_j^{k+1} + C_{j-1}^{k+1}) - Q (0.5C_{j+1}^{k+1} - 0.5C_{j-1}^{k+1}) \quad (\text{B-151})$$

Collecting terms, this equation can be rewritten as:

$$\frac{M_j^{k+1} - M_j^k}{\Delta t} = C_j^{k+1} \left[ Q \left( -2 \frac{\alpha n}{L} \right) \right] + C_{j-1}^{k+1} \left[ Q \left( \frac{\alpha n}{L} + 0.5 \right) \right] + C_{j+1}^{k+1} \left[ Q \left( \frac{\alpha n}{L} - 0.5 \right) \right] \quad (\text{B-152})$$

Finally, using (B-143), we get the following:

$$\begin{aligned} \frac{M_j^{k+1} - M_j^k}{\Delta t} = & -C_j^{k+1}[Q(1 + 2 * DispFactor)] \\ & + C_{j-1}^{k+1}[Q(1 + DispFactor)] \\ & + C_{j+1}^{k+1}[Q(DispFactor)] \end{aligned} \tag{B-153}$$

Simplifying this equation (by focusing on a particular Cell in our example, say Cell2, and ignoring the superscripts for time), we find that the rate of change of mass in a particular Cell in the Aquifer element (in this case, Cell2), accounting for both advection and dispersion, can be approximated as follows:

$$\begin{aligned} \text{Mass Rate of Change in Cell2} = & - C_2 * Q(1 + 2 * DispFactor) \\ & + C_1 * Q(1 + DispFactor) \\ & + C_3 * Q(DispFactor) \end{aligned} \tag{B-154}$$

We can now see what the various Outflows that GoldSim automatically created represent. The first term represents the mass flows leaving Cell2. This consists of the advective flow downstream to Cell3 (equal to  $Q * C_2$ ) and two dispersive flows (equal to  $Q * C_2 * DispFactor$ ), one upstream to Cell2 and one downstream to Cell3.

The second term is the mass flow entering Cell2 from Cell1 (an advective flow equal to  $Q * C_1$  and a dispersive flow equal to  $Q * C_1 * DispFactor$ ).

The third term is the mass flow entering Cell2 from Cell3 (a dispersive flow equal to  $Q * C_3 * DispFactor$ ).

This approximation is accurate to the second order with respect to the spatial discretization.

Even in the absence of the dispersive terms, a network of linked Cells simulating advective transport will inevitably exhibit a degree of *numerical dispersion* that is a function of the number of Cells (the degree of discretization). In particular, the equivalent numerical dispersivity is equal to  $\Delta x / 2$ . As a result, if the number of Cells is less than the pathway length divided by twice the dispersivity, that is,  $n < L / (2\alpha)$ , then the numerical dispersivity will exceed the specified dispersivity. If this occurs, GoldSim records a warning in the Run Log (indicating that you either need to use more Cells or increase the dispersivity to accurately model longitudinal dispersion along the pathway).

The dispersive term in Equation (B-144) should actually also include molecular diffusion. That is the equation should look like this:

$$\frac{\partial C}{\partial t} = (D + D_m) \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \tag{B-155}$$

Where  $D_m$  is the molecular diffusion coefficient. That is, the impact of molecular diffusion is not represented in (B-154). To account for the effect of molecular diffusion on the longitudinal dispersion, GoldSim also automatically adds diffusive connections between the Cells (which in most cases is likely to be negligible).

## Network Pathway Details

Network pathways provide a computationally efficient way to simulate large, complex networks of one-dimensional conduits in order to describe contaminant transport through fractured rock systems.

The ability to solve Network pathways efficiently results from the fact that it is possible to develop a Laplace-transformed transfer matrix for an entire network of Pipe pathways by simple additions and multiplications of the transformed transfer matrices for each individual pathway (Barten, 1996). Once the network transfer matrix/matrices are developed, then the transport calculations for the network are no more time-consuming than for a single Pipe pathway. The only extra computational expense required is the time required for the creation of the network transfer matrix at the beginning of the simulation. For even quite large networks (100,000 pipes or more), this time is not excessive.

### Developing a Transfer Matrix for a Network of Pipes

GoldSim's boundary condition for pipes assumes that the pipe extends infinitely, and has concentrations of zero at plus and minus infinity. Mass is then injected into the upstream end of the pipe. Using this assumption, GoldSim calculates the discharge mass flux at the true end of the pipe. In other words, the discharge is calculated as if the pipe did not 'see' its ends.

When a Network pathway is defined in GoldSim, the calculated outflux from each pipe is applied as the influx to each connected downstream pipe. There is no attempt to maintain continuity of concentrations at the pipe connections, only continuity of the mass flux.

The manner in which GoldSim uses Laplace-transformed transfer matrices to convert mass-influx to mass-outflux histories for pipes is described in detail in "Solution Technique for Pipe Pathways".

**Read more:** [Solution Technique for Pipe Pathways](#) (page 358).

Multiplying a transfer matrix by a transformed influx history produces a transformed outflux history. When calculating the transfer matrix for an entire pipe network, GoldSim uses the following rules:

- Where two pipes in a network are connected in series, their combined behavior is defined by the product of their transfer matrices.
- When a pipe splits into two (or more) downstream pipes, each has a transfer matrix defined by the product of the upstream pipe's transfer matrix with the downstream pipe's transfer matrix, multiplied by the fraction of flow going into the downstream pipe.
- When two (or more) pipes merge, their transfer matrices are simply summed.

GoldSim uses the above rules to create a "total" transfer matrix for each source-sink combination in the network. If there were two sources, and three sinks in the network, GoldSim would calculate six transfer matrices. (Actually, there are separate transfer matrices for each radionuclide decay chain. GoldSim handles these internally, so the user is not aware of the details).

## References

The references cited in this appendix are listed below:

- Barker, J., 1985, "Block Geometry Functions Characterizing Transport In Densely Fissured Media", *J. Hydrology*, 77 (1985), pp. 263-279.

Barten, W., 1996, "Linear Response Concept Combining Advection And Limited Rock Matrix Diffusion In A Fracture Network Transport Model", Water Resources Research, 32(11), pp. 3285-3296, 1996.

de Hoog, F. R., J. H. Knight, and A. N. Stokes, 1982, "An Improved Method for Numerical Inversion of Laplace Transforms", SIAM J. Sci. Stat. Comput., Vol. 3, No. 3, Sept. 1982.

---

# Appendix C: Implementing External (DLL) Pathways

The order of operations “putting your socks on” and “putting your shoes on” is of practical importance.

John Addison

## Appendix Overview

External Pathways provide a mechanism by which external functions for contaminant transport (e.g., analytical, finite element or finite difference solute transport models) can be directly integrated into GoldSim.

Integrating external contaminant transport functions into GoldSim requires that you develop a “wrapper” (or “shell”) around your existing function, and compile it into a DLL.

Note that External Pathways are specialized extensions of External elements. Hence, before reading this appendix, you should refer first to Appendix C of the **GoldSim User’s Guide**, “Implementing External (DLL) Elements”, which describes in general how external functions must be coded and compiled. The current appendix provides additional details regarding creating external functions which represent contaminant transport pathways.

### In this Appendix

This appendix includes the following two sections:

- Details of External Pathway Functions
- External Pathway Function Example

## Details of External Pathway Functions

An external function which is used to represent contaminant transport is referred to as an *external pathway function*. An external pathway function is a specialized type of external function. As such, it must have the same properties and behave in the same manner as other external functions (as described in Appendix C of the **GoldSim User's Guide**, "Implementing External (DLL) Elements").

### Special Requirements for External Pathway Function Input/Output Argument Lists

In addition to having all the characteristics of an external function, external pathway functions must also receive as input and return as output vectors of species mass. Hence, external pathway functions have the following specialized requirements (beyond those required for all external functions):

- The first input argument to the external function should normally be "Etime" (elapsed time of the run). The user may provide any number of additional input arguments after Etime, such as material properties or climatic variables, or a pathway-specific index. As an example, the user could pass a flag indicating the location of the pathway in a groundwater flow network. This information could be used by the external function as an index to identify the pathway which is represented, and decide which external data files to read in. In this way, an external function can service multiple pathways.
- At each update of the system, the input arguments followed by the mass transfer arguments are passed to the external function with Xfmethod = XF\_CALCULATION. For this call, the input argument-list provided to the function will *automatically* have the following items added to it after the user-specified parameters by GoldSim:
  - the number of species in each buffer;
  - a flag equal to 1.0 if the input buffer is non-zero, and 0.0 otherwise (this allows the external pathway function to skip time-consuming calculations until it receives its first mass input);
  - the number of input buffers (which will be 1 if the "Combine flux inputs to pathway" option is true, and otherwise will equal the number of influx mass flux links). "Combine flux inputs to pathway" tells GoldSim to merge all influxes to the pathway, and present the external function with a single combined input mass buffer;
  - the number of output buffers (which will be 1 if the "Split single flux output from pathway" option is true, and otherwise will equal the number of outflux mass flux links). "Split single flux output from pathway" tells GoldSim that the external function calculates a single output buffer, and that GoldSim should divide it amongst all outfluxes in proportion to their flow rates; and
  - {(number of input buffers) \* (number of species)} values representing the masses of species (in kilograms) to be input to the function. (The order in which the species mass is passed is described below).
- The function must return any user-specified outputs followed by one or more discharge-buffers in its output argument list. If the "Split single flux output from pathway" option is true, then the model returns a

## Passing Mass Between GoldSim and the External Pathway Function

single discharge buffer which GoldSim divides amongst all of its outflux mass flux links proportionately to their flow rates. If the “Split single flux output from pathway” option is false, the model returns an output buffer for each outflux from the pathway.

Each input and discharge buffer passes species according to the order the species are listed in the Species element. Data are passed from and to GoldSim one buffer at a time (i.e., all species are passed for the 1<sup>st</sup> buffer, then all species are passed for the second buffer, etc.).

Input mass buffers (mass vectors which are sent *to* the external pathway function from GoldSim) are passed according to the following rules:

- If the “Combine flux inputs to path” option is checked, a single mass buffer is sent to the external pathway function, combining all of the influxes to the pathway, as well as any mass associated with an initial/boundary condition.
- If the “Combine flux inputs to path” option is not checked, a separate mass buffer is sent for each influx to the pathway. Advective influxes are sent first (in the order they are listed in the Inflows tab for the pathway), followed by diffusive influxes (in the order they are listed in the Diffusive Fluxes tab for the pathway). Initial/boundary conditions are added to the first advective influx (or the first diffusive influx in the absence of advective influxes).

Output mass buffers (mass vectors which are sent *from* the external pathway function back to GoldSim) are treated according to the following rules:

- If the “Split single flux output from pathway” option is checked, a single mass buffer is sent from the external pathway function, and GoldSim divides it amongst all outfluxes in proportion to their flow rates. (Note that you can only create advective outfluxes from an External Pathway; diffusive outfluxes cannot be created).
- If the “Split single flux output from pathway” option is not checked, a separate mass buffer **MUST BE SENT** from the external function to GoldSim for each outflux from the pathway. The buffers are assigned to each advective outflux in the order they are listed in the Outflows tab for the pathway.

## Additional Comments on External Pathway Functions

Several other points regarding the use and behavior of external pathway functions should be noted:

- You can send uncertain parameters as arguments to external pathway functions, allowing the function to take advantage of GoldSim’s powerful Monte Carlo simulation framework.
- The properties of external pathway functions can change with time, since GoldSim will always pass the current values of any specified input parameters to the external pathway function. For example, if the annual precipitation rate was a time-varying parameter in GoldSim, and it was passed to the external pathway function, the function could update its flow field appropriately.
- The external function is expected to initialize itself if necessary (and read any necessary external files). The function is also expected to keep track of the “previous” value of time passed to it by GoldSim. At each call, the external pathway function must carry forward its calculations up to the current time, and return the incremental masses discharged.

## External Pathway Function Example

An example C listing for an external pathway function is provided below.

```
// Utility method used to simplify the sending of an error message to GoldSim
// (see Appendix C of GoldSim User's Guide for the implementation).
extern void CopyMsgToOutputs(const char* sMessage, double* outargs);

// Global enumerations, useful for C-style implementations
//
// XFMethodID identifies the method types, used to identify the phase of the simulation
// that is currently in progress.
//
//     XF_INITIALIZE    - Called after DLL is loaded and before each realization.
//     XF_CALCULATE     - Called during the simulation, each time the inputs change.
//     XF_REP_VERSION   - Called after DLL load to report the external fcn version number.
//     XF_REP_ARGUMENTS - Called after DLL load to report the number of input and output
//                       arguments.
//     XF_CLEANUP       - Called before the DLL is unloaded.
//
enum XFMethodID
{
    XF_INITIALIZE = 0, XF_CALCULATE = 1, XF_REP_VERSION = 2, XF_REP_ARGUMENTS = 3,
    XF_CLEANUP = 99
};

// XFStatusID identifies the return codes for external functions.
//
//     XF_SUCCESS        - Call completed successfully.
//     XF_CLEANUP_NOW    - Call was successful, but GoldSim should clean up
//                       and unload the DLL immediately.
//     XF_FAILURE        - Failure (no error information returned).
//     XF_FAILURE_WITH_MSG - Failure, with DLL-supplied error message available.
//                       Address of error message is returned in the first element
//                       of the output arguments array.
//     XF_INCREASE_MEMORY - Failed because the memory allocated for output arguments
//                       is too small. GoldSim will increase the size of the
//                       output argument array and try again.
//
enum XFStatusID
{
    XF_SUCCESS = 0, XF_FAILURE = 1, XF_CLEANUP_NOW = 99, XF_FAILURE_WITH_MSG = -1,
    XF_INCREASE_MEMORY = -2
};

// Helper function used to perform XF_CALCULATION step for ExtPathwaySum
int ExtPathSumCalc(const double* inargs, double* outargs)
{
    const double time = inargs[0]; // time to calculate up to
    const double factor = inargs[1]; // multiplication factor

    if (factor <= 0)
    {
        CopyMsgToOutputs("Error: multiplication factor is non-positive!", outargs);
        return XF_FAILURE_WITH_MSG;
    }

    outargs[0] = time;
    outargs[1] = time*factor;
    const int nrn = (int) inargs[2]; // number of species per buffer
    const int input = (int) inargs[3]; // anything in the input buffer?
    const int ninbufs = (int) inargs[4]; // number of input buffers
    const int noutbufs = (int) inargs[5]; // number of output buffers

    if (noutbufs <= 0)
        return XF_SUCCESS;

    for (int i=0; i < nrn; ++i)
    {
```

```

// Add the input buffers
double totin = (double) 0.0;
for (int j=0; j < ninbufs; ++j)
    totin += inargs[6 + j*nrn + i];

// Divide the result among the output buffers
double outval = factor*totin/noutbufs;
for (int j=0; j < noutbufs; ++j)
    outargs[2 + j*nrn + i] = outval;
}
return XF_SUCCESS;
}

////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
// ExtPathwaySum
// External Pathway element example. Takes the sum of all inflows,
// multiplies by a user-supplied factor, and divides the result
// among the outflows.
//
extern "C" void __declspec(dllexport) ExtPathwaySum(const int      methodID,
                                                    int*          status,
                                                    const double* inargs,
                                                    double*          outargs)
{
    static const double VERSION = 4.21;    // Version number
    static const double INPUTS  = 2.0;    // Number of inputs expected.
    static const double OUTPUTS = 2.0;    // Number of outputs returned.
    *status = XF_SUCCESS;
    switch (methodID)
    {
    case XF_INITIALIZE:
        break; // nothing required
    case XF_REP_VERSION:
        outargs[0] = VERSION;
        break;
    case XF_REP_ARGUMENTS:
        outargs[0] = INPUTS;
        outargs[1] = OUTPUTS;
        break;
    case XF_CALCULATE:
        *status = ExtPathSumCalc(inargs, outargs);
        break;
    case XF_CLEANUP:
        break;
    default:
        *status = XF_FAILURE_WITH_MSG;
        CopyMsgToOutputs("Unknown method ID requested", outargs);
        break;
    }
}
}

```

The following code is the same algorithm, implemented in Intel Visual Fortran.

```

! Utility module to specify the GoldSim parameter constants
module gs_parameters
    implicit none

    ! Parameters to identify the method types, which indicate the phase of the
    ! simulation that is currently in progress.
    !
    ! INITIALIZE      - Called after DLL is loaded and before each realization.
    ! CALCULATE      - Called during the simulation, each time the inputs change.
    ! REPORT_VERSION  - Called after DLL load to report the external fcn version number.
    ! REPORT_ARGUMENTS - Called after DLL load to report the number of input and output
    !                  arguments.
    ! CLEANUP        - Called before the DLL is unloaded.

    integer(4), parameter :: INITIALIZE      = 0

```

```

integer(4), parameter :: CALCULATE      = 1
integer(4), parameter :: REPORT_VERSION = 2
integer(4), parameter :: REPORT_ARGUMENTS = 3
integer(4), parameter :: CLEANUP       = 99

! Parameters to identify the return codes for external functions.
!
! SUCCESS          - Call completed successfully.
! CLEANUP_NOW      - Call was successful, but GoldSim should clean up
!                  and unload the DLL immediately.
! FAILURE          - Failure (no error information returned).
! FAILURE_WITH_MSG - Failure, with DLL-supplied error message available.
!                  Address of error message is returned in the first element
!                  of the output arguments array.
! INCREASE_MEMORY  - Failed because the memory allocated for output arguments
!                  is too small. GoldSim will increase the size of the
!                  output argument array and try again.

integer(4), parameter :: SUCCESS          = 0
integer(4), parameter :: FAILURE          = 1
integer(4), parameter :: CLEANUP_NOW      = 99
integer(4), parameter :: FAILURE_WITH_MSG = -1
integer(4), parameter :: INCREASE_MEMORY  = -2

end module gs_parameters

! external copy_msg_to_outputs
! Utility subroutine used to simplify the sending of an error message to GoldSim
! (see Appendix C of GoldSim User's Guide for the implementation).

! Helper function called from ext_pathway_sum to do the calculation work.
integer(4) function ext_path_sum_calc(inargs, outargs)
  use gs_parameters
  implicit none
  real(8) inargs(*), outargs(*)
  integer(4) nrn, ninbufs, noutbufs, i, j
  real(8) dtime, dfactor, dtotin, doutval

  dtime = inargs(1)
  dfactor = inargs(2)

  if (dfactor .le. 0) then
    call copy_msg_to_outputs('Error: multiplication factor is non-positive!', &
                             outargs)
    ext_path_sum_calc = FAILURE_WITH_MSG
    return
  end if

  outargs(1) = dtime
  outargs(2) = dtime*dfactor
  nrn = int(inargs(3)) ! number of species per buffer
  ninbufs = int(inargs(5)) ! number of input buffers
  noutbufs = int(inargs(6)) ! number of output buffers

  if (noutbufs .le. 0) then
    ext_path_sum_calc = SUCCESS
    return
  end if

  do i = 1, nrn
    ! Add the input buffers
    dtotin = 0.0
    do j = 1, ninbufs
      dtotin = dtotin + inargs(6 + (j-1)*nrn + i)
    end do

    ! Divide the result among the output buffers
    doutval = dfactor*dtotin/noutbufs
    do j = 1, noutbufs
      outargs(2 + (j-1)*nrn + i) = doutval
    end do
  end do
end function

```

```

        end do

        ext_path_sum_calc = SUCCESS
    end function ext_path_sum_calc

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! ext_pathway_sum
!   External Pathway element example. Takes the sum of all inputs,
!   multiplies by a user-supplied factor, and divides the result
!   among the outputs.
!
subroutine ext_pathway_sum(method_id, status, inargs, outargs)
!DEC$ ATTRIBUTES dllexport,c :: ext_pathway_sum
!DEC$ ATTRIBUTES value      :: method_id
!DEC$ ATTRIBUTES reference  :: status
!DEC$ ATTRIBUTES reference  :: inargs
!DEC$ ATTRIBUTES reference  :: outargs

use gs_parameters
implicit none
real(8),    parameter :: VERSION = 4.21 // Version number.
integer(4), parameter :: NINPUTS  = 2  // Number of inputs expected.
integer(4), parameter :: NOUTPUTS = 2  // Number of outputs returned.

integer(4) method_id, status
real(8)    inargs(*), outargs(*)
integer(4) ext_path_sum_calc

select case (method_id)
case (INITIALIZE)
    status = SUCCESS
case (REPORT_VERSION)
    outargs(1) = VERSION
    status = SUCCESS
case (REPORT_ARGUMENTS)
    outargs(1) = NINPUTS
    outargs(2) = NOUTPUTS
    status = SUCCESS
case (CALCULATE)
    status = ext_path_sum_calc(inargs, outargs)
case (CLEANUP)
    status = SUCCESS
case default
    call copy_msg_to_outputs('Unknown method ID requested', outargs)
    status = FAILURE_WITH_MSG
end select

end subroutine ext_pathway_sum

```



---

# Appendix D: Network Pathway File Format

There are three kinds of lies: lies, damned lies, and statistics.

Benjamin Disraeli

## Appendix Overview

Network Pathways use a Laplace-transform approach to provide a computationally efficient way to simulate large, complex networks of one-dimensional conduits in order to describe contaminant transport through fractured rock systems

Network Pathways require specification of a *fracture network*, which identifies all of the pipes in the network, the manner in which they are connected, and each pipe's geometry and flow rate. The fracture network can be entered by hand, but more likely, would be generated (based on a statistical description of the fracture system) by a discrete fracture generation and flow simulation code and read into GoldSim as a text file. This appendix describes the format for such a file.

# Fracture Network File Format

The fracture network file is expected to have the extension “.LTX”, although this is not required. This is a text file.

The file has six sections. Each section starts with a BEGIN and ends with an END record. All records outside of these six sections are treated as comments, and ignored. Numbers can be separated by spaces or commas. Each record in the file can consist of up to 5000 characters. A "+" sign can be added to a record to indicate that it is continued on the following record.

The format for each section is as follows:

1. Definition of the “pipes”:

Starts with “BEGIN PIPES nnn”, where nnn is the total number of pipes. Has one record per pipe, containing:

- pipe-number (starting from 1),
- length (m),
- flow rate (m<sup>3</sup>/yr),
- flowing cross-sectional area (m<sup>2</sup>),
- wetted surface area (m<sup>2</sup>) which is the perimeter multiplied by the pipe length,
- transmissivity (m<sup>2</sup>/yr), which is ignored by GoldSim,
- external index for the pipe, which is ignored by GoldSim, and
- fracture set ID for the pipe, which must correspond to a GoldSim fracture set ID.

Ends with an END record.

2. Definition of Source Groups:

Starts with a record “BEGIN source\_groups”.

Contains any number of source-group sets. Each set starts with its ID, the number of pipes in the set, and then the pipe numbers. Note that if these records are lengthy, a + sign may be used to continue onto another record.

The group ID must correspond to a GoldSim pathway which is connected into the fracture network, unless the GoldSim option to combine inputs was selected, in which case the source group ID is ignored. If there are no input connections to the network, and its source-term is defined by an initial/boundary specification, the source group ID must be “-source-”.

**Read more:** [Combining and Splitting Fluxes to Create Single Sources and Sinks](#) (page 239); [Defining Initial/Boundary Conditions for a Network Pathway](#) (page 239).

Note that influxes of species to the source group are distributed by GoldSim to individual pipes in proportion to their flow rates.

Ends with an END record.

3. Definition of Sink Groups:

Starts with a record “BEGIN sink\_groups”.

Contains any number of sink-group sets. Each set starts with its ID, the number of pipes in the set, and then the pipe numbers. Note that if these records are lengthy, a + sign may be used to continue onto another record.

The group ID must correspond to a GoldSim pathway which is connected as an output from the fracture network, unless the GoldSim option to merge outputs was selected, in which case the sink group ID is ignored.

Ends with an END record.

4. Definition of Watch Groups (optional):

Starts with a record "BEGIN watch\_groups".

Contains up to 99 watch group sets. Each set starts with its group ID (in the form Watch $nn$ , where  $nn$  is a number between 01 and 99). This is followed by the number of pipes whose discharges are to be included in the watch group, and then the pipe numbers.

Ends with an END record.

5. Definition of Upstream pipes:

Starts with a record "BEGIN upstream\_connections".

For each pipe, has a record starting with the pipe-number, followed by the numbers of all upstream pipes. A maximum of 1000 upstream pipes can be defined. Note that if these records are lengthy, a + sign may be used to continue onto another record.

Ends with an END record.

6. Definition of Downstream pipes:

Starts with a record "BEGIN downstream\_connections".

For each pipe, has a record starting with the pipe-number, followed by the numbers of all downstream pipes. A maximum of 1000 downstream pipes can be defined. Note that if these records are lengthy, a + sign may be used to continue onto another record.

Ends with an END record.

The following is an example of a fracture network file for a 26-pipe system.

```
BEGIN pipes 26
    1, 20, 0.81917, 0.00964563, 610, 1e-007, 0, "SET_1"
    2, 20, 0.87987, 0.0127828, 808.4, 1e-007, 1, "SET_1"
    3, 20, 1.30806, 0.017457, 1104, 1e-007, 3, "SET_1"
    4, 20, 1.73638, 0.017888, 800, 2e-007, 4, "SET_1"
    5, 20, 2.85418, 0.0236569, 1058, 2e-007, 5, "SET_1"
    6, 20, 1.19785, 0.0121191, 542, 2e-007, 6, "SET_1"
    7, 20, 3.44909, 0.0253, 800, 4e-007, 7, "SET_1"
    8, 20, 3.00444, 0.0171407, 542, 4e-007, 8, "SET_1"
    9, 20, 3.89948, 0.0305751, 966.8, 4e-007, 9, "SET_1"
    10, 20, 7.30741, 0.0381773, 853.6, 8e-007, 10, "SET_2"
    11, 20, 6.96732, 0.0404672, 904.8, 8e-007, 11, "SET_2"
    12, 20, 6.69494, 0.0250818, 560.8, 8e-007, 12, "SET_2"
    13, 20, 10.8668, 0.14176, 708.8, 1.6e-005, 14, "SET_2"
    14, 20, 12.0651, 0.1808, 904, 1.6e-005, 15, "SET_2"
    15, 20, 6.96720, 0.18144, 907.2, 1.6e-005, 16, "SET_2"
    16, 20, 13.3724, 0.29856, 1492.8, 1.6e-005, 17, "SET_2"
    17, 20, 0.33966, 0.19288, 964.4, 1.6e-005, 18, "SET_1"
    18, 20, 0.11009, 0.16, 800, 1.6e-005, 19, "SET_1"
    19, 20, 0.42806, 0.1484, 742, 1.6e-005, 20, "SET_1"
    20, 20, 1.05681, 0.16, 800, 1.6e-005, 21, "SET_1"
    21, 20, 0.61247, 0.13784, 689.2, 1.6e-005, 22, "SET_1"
    22, 20, 0.06071, 0.17328, 866.4, 1.6e-005, 23, "SET_1"
    23, 20, 6.67778, 0.08272, 413.6, 1.6e-005, 24, "SET_2"
    24, 20, 3.67335, 0.16, 800, 1.6e-005, 25, "SET_2"
    25, 20, 13.3727, 0.1224, 612, 1.6e-005, 26, "SET_2"
    26, 20, 0.81921, 0.16032, 801.6, 1.6e-005, 27, "SET_2"
END

BEGIN source_groups
    "BG1", 1, 16
END

BEGIN sink_groups
    "BG2", 1, 25
END

BEGIN upstream_connections
    1, 2
    2, 3
    3, 16
    4, 6, 18, 19
    5, 4, 20, 22
```

```
6, 14
7, 9
8, 7, 21
9, 13
10, 11, 17
11, 15
12, 10
13, 14
14, 16
15, 13
16
17, 9
18, 9
19, 3
20, 7, 21
21, 10
22, 2
23, 8, 24
24, 5, 26
25, 12, 23
26, 1
```

END

BEGIN downstream\_connections

```
1, 26
2, 1, 22
3, 2, 19
4, 5
5, 24
6, 4
7, 8, 20
8, 23
9, 7, 17, 18
10, 12, 21
11, 10
12, 25
13, 9, 15
14, 6, 13
15, 11
16, 3, 14
17, 10
18, 4
19, 4
20, 5
```

21, 8, 20

22, 5

23, 25

24, 23

25

26, 24

END

---

# Appendix E: Details of Source Computations

*Student:* Professor, are you sure that the derivation of that equation is “obvious”?

*Professor* (after staring at the board, leaving the classroom, and returning 15 minutes later): Yes.

Exchange in Freshman Calculus class,  
University of Michigan

## Appendix Overview

This appendix presents the theoretical basis and the mathematical details of contaminant Sources in GoldSim. Because the key assumptions upon which the behavior of Sources is based are presented in the main text (Chapter 5), an understanding of these details is not necessary in order to use the Contaminant Transport Module. Nevertheless, many experienced modelers will want to have a more detailed understanding of the equations upon which the Sources are based, and that information is presented in this appendix.

### In this Appendix

This appendix includes the following:

- Barrier Failure Distributions
- Combining Failure Modes
- Computing Exposure Rates

## Barrier Failure Distributions

GoldSim allows you to simulate the failure of any barriers surrounding contaminants in a Source by defining *failure distributions*. A failure distribution is a density function of failure frequency.

**Read more:** [Defining Barrier Failure](#) (page 271).

GoldSim allows you to define the failure distributions using one of six distributions:

- Immediate;
- Uniform;
- Weibull;
- Exponential;
- User-Defined; or
- Table.

The mathematical details of these distributions are discussed below. In the equations presented below,  $f(t)$  represents the density function (the fractional failure rate) as a function of time, while  $F(t)$  represents the cumulative distribution function (the cumulative fraction of failed barriers) as a function of time.

### Immediate Failure Distribution

The Immediate failure distribution is the simplest of the failure distributions. All containers fail immediately when the distribution begins. That is, all its probability density is concentrated at a single value. Mathematically,

$$\begin{aligned} F(t) &= 0 && \text{for } t < t_{\text{fail}} \\ F(t) &= 1 && \text{for } t \geq t_{\text{fail}} \end{aligned} \quad (\text{E-1})$$

where  $t_{\text{fail}}$  is the time at which the distribution begins (Effective Time = 0).

### Uniform Failure Distribution

The Uniform failure distribution is used when the failure rate is assumed to be uniform (constant) over time.

The failure rate is computed as follows:

$$f(t) = \frac{1}{b - a} \quad (\text{E-2})$$

where  $a$  is the time that failure starts, and  $b$  is the time that failure ends. Hence,  $b - a$  is the duration of the failure distribution.

The fraction failed is therefore:

$$\begin{aligned} F(t) &= 0 && \text{for } t \leq a \\ F(t) &= \frac{t - a}{b - a} && \text{for } a \leq t \leq b \\ F(t) &= 1 && \text{for } t \geq b \end{aligned} \quad (\text{E-3})$$

### Weibull Failure Distribution

The Weibull failure distribution is often used to characterize failure times in reliability models. It is defined by a minimum value ( $\epsilon$ ), a scale parameter ( $\beta$ ), and a slope or shape parameter ( $\alpha$ ).

The failure rate is computed as follows:

$$f(t) = \frac{\alpha}{\beta - \varepsilon} \left( \frac{t - \varepsilon}{\beta - \varepsilon} \right)^{\alpha-1} e^{-\left( \frac{t - \varepsilon}{\beta - \varepsilon} \right)^\alpha}$$

(E-4)

The fraction failed is then:

$$F(t) = 1 - e^{-\left( \frac{t - \varepsilon}{\beta - \varepsilon} \right)^\alpha} \quad (E-5)$$

Note that in GoldSim, rather than specifying the scale parameter ( $\beta$ ), the user specifies a *mean lifetime* ( $\mu$ ). GoldSim converts the mean lifetime to the scale parameter as follows:

$$\beta = \frac{\mu}{\Gamma\left(1 + \frac{1}{\alpha}\right)} \quad (E-6)$$

### Exponential Failure Distribution

The exponential failure distribution is described by a single parameter,  $\lambda$ . This represents the inverse of the expected lifetime.

The failure rate is computed as:

$$f(t) = \lambda e^{-\lambda t} \quad (E-7)$$

The fraction failed is then:

$$F(t) = 1 - e^{-\lambda t} \quad (E-8)$$

### User-Defined and Table Failure Distributions

Both of these distributions simply provide a mechanism by which the user specifies the fraction failed,  $F(t)$ , directly as a function of the effective time. For a User-Defined distribution, an equation representing  $F(t)$  is entered. For a Table distribution, a 1-D table created by an external function is used to define  $F(t)$ .

## Combining Failure Modes

For a particular barrier, multiple *failure modes* can be defined, with each mode having a different failure distribution.

**Read more:** [Defining Barrier Failure](#) (page 271).

For example, one failure mode may be assigned to represent one type of corrosion (e.g., uniform corrosion), while another may be assigned to represent another type of corrosion (e.g., pitting corrosion). GoldSim combines the failure modes in an appropriate manner to obtain the total failure distribution. It is assumed that the different modes operate independently and without synergism. This section describes the manner in which the separate failure modes are mathematically combined.

Let

- N = number of failure modes;
- $f_i(t)$  = frequency (rate) of failure by mode  $i$  at time  $t$ ;
- $F_i(t)$  = probability of failure (fraction of barriers failed) by mode  $i$  at time  $t$ ;
- $p_i$  = fraction of containers which can fail by mode  $i$ ;
- $f(t)$  = frequency of failure by all modes combined at time  $t$ ; and

$F(t)$  = probability of failure (fraction of barriers failed) by all modes combined at time  $t$ .

By definition, for a single failure mode:

$$F_i(t) = \int_0^t f_i(\theta) d\theta \quad (E-9)$$

and for all failure modes combined:

$$F(t) = \int_0^t f(\theta) d\theta \quad (E-10)$$

We would like to develop an expression such that the combined distributions  $f(t)$  and  $F(t)$  can be expressed in terms of the distributions for the modes,  $f_i(t)$  and  $F_i(t)$ . The derivation is straightforward.

$$1 - p_i F_i(t) = \text{probability of surviving mode } i \text{ by time } t \quad (E-11)$$

Assuming that the failure modes are uncorrelated, it follows that

$$\prod_{i=1}^n [1 - p_i F_i(t)] = \text{probability of surviving all modes by time } t \quad (E-12)$$

and

$$F(t) = 1 - \prod_{i=1}^n [1 - p_i F_i(t)] = \text{probability of not surviving all modes by time } t \quad (E-13)$$

Hence, GoldSim uses Equation (E-13) to combine multiple failure modes into a single combined failure distribution.

## Computing Exposure Rates

GoldSim explicitly represents two processes which control release of mass from a Source:

1. *exposure* of the contaminant mass within a Source; and
2. *transport* of exposed contaminant mass through and away from the Source.

**Read more:** [Processes Modeled by a Source](#) (page 261).

The second process is simulated using GoldSim's Cell pathways. The Cell pathway equations and algorithms are discussed in detail in Appendix B.

**Read more:** [Appendix B: Details of Pathway Computations](#) (page 315).

The first process, exposure of the contaminant mass within the Source, is discussed in detail in this section.

### Understanding Exposure

The term *exposure*, as applied to a Source, has a specific meaning within GoldSim. In particular, species mass in a Source is considered to be *exposed* if it is available for mass transfer within and away from the Source. If a contaminant is present within an intact barrier, or bound within intact matrix material of some sort (e.g., grout, metal, glass), it is not available for mass transport, and hence is considered to be *unexposed*. The mass cannot be transported until it is physically liberated from barriers and/or matrix material

present at the Source. Hence, within a Source, exposure is controlled by two processes:

- *Loss of Containment.* The mass can be specified to be present in the Source in discrete *packages* (e.g., 100 separate drums). For each individual package, up to two layers of containment (barriers) can be explicitly considered to exist (e.g., a drum and a liner within the drum). The mass can be distributed in one of two different places within the barrier system in a package (between the outer and inner barriers, or inside both barriers). Barrier failure rates are described by the user in terms of density functions of failure frequency (e.g., the rate of drum failure).
- *Degradation of waste matrix.* All or portions of the species mass within the Source can be specified to exist within one or more matrix materials, such as cement, grout, solidified glass, or metal. Species which are bound in such a matrix are not released until the matrix itself degrades (e.g., dissolves, corrodes or alters) in some manner. Release of species mass from the matrix is then assumed to be congruent with the degradation of the matrix. Degradation rates are specified directly by the user.

These two processes together determine the *rate of exposure* of contaminant mass within a Source. The manner in which exposure rates are computed by GoldSim is described below.

## Calculating the Exposure Rate for a Source

You can define multiple inventories for each Source, and a particular inventory exists in one of three locations:

- Inside the outer barrier and outside of the secondary barrier, but not bound within a waste matrix. In the discussion that follows, this is referred to as an “outer” inventory.
- Inside the inner barrier, but not bound within a waste matrix. In the discussion that follows, this is referred to as an “inner” inventory.
- Bound within a waste matrix which is either 1) inside the outer barrier; 2) inside both the outer barrier and inner barrier; or 3) not surrounded by a barrier (if no barriers are defined for the Source). In the discussion that follows, this is referred to as a “bound” inventory.

**Read more:** [Defining Source Inventories](#) (page 265).

Since each of these three types of inventories is exposed in a different manner, it is necessary to compute the exposure rate for species *n* at time *t* for each type separately and sum these values to obtain the total exposure rate:

$$e(n, t) = \sum_{q=1}^{NI_q} e_{q,o}(n, t) + \sum_{r=1}^{NI_r} e_{r,i}(n, t) + \sum_{s=1}^{NI_s} e_{s,b}(n, t) \quad (E-14)$$

where:

- $e(n, t)$  = the total exposure rate for species *n* in the Source at time *t* [M/T];
- $e_{q,o}(n, t)$  = the exposure rate for species *n* in outer inventory *q* for the Source at time *t* [M/T];
- $e_{r,i}(n, t)$  = the exposure rate for species *n* in inner inventory *r* for the Source at time *t* [M/T];

$e_{s,b}(n,t)$  = the exposure rate for species  $n$  in bound inventory  $s$  for the Source at time  $t$  [M/T];

$NI_q$  = number of outer inventories for the Source;

$NI_r$  = number of inner inventories for the Source; and

$NI_a$  = number of bound inventories for the Source.

These components can be computed as functions of the following parameters:

$c(t)$  = outer barrier failure rate at time  $t$  [1/T];

$w(t,\theta)$  = inner barrier failure rate at time  $t$  for an outer barrier that has failed at time  $\theta$  [1/T]

$I_q(n,t)$  = mass of species  $n$  *per unfailed package* in outer inventory  $q$  at time [M];

$I_r(n,t)$  = mass of species  $n$  *per unfailed package* in inner inventory  $r$  at time [M];

$I_s(n,t)$  = mass of species  $n$  *per unfailed package* in bound inventory  $s$  at time [M];

$k_s(t)$  = fractional degradation rate of waste matrix for bound inventory  $s$  [1/T]; and

$N$  = number of packages in the Source.

$c(t)$  and  $w(t, \theta)$  are the barrier failure distributions.

**Read more:** [Defining Barrier Failure](#) (page 271).

Note that for a given Source, all inventories are controlled by the same inner and outer barrier failure distributions.

$I_q(n,t)$ ,  $I_r(n,t)$ , and  $I_s(n,t)$  define the species mass in an *unfailed* package for each inventory. Note that these masses may change with time due to decay processes (some species decreasing and others increasing due to the production of daughter products).

$k_s(t)$  is the degradation rate of the waste matrix.

**Read more:** [Specifying an Inventory](#) (page 265).

### Exposure Rate for Outer Inventories

The exposure rate for those inventories that are exposed instantaneously upon outer barrier failure is directly proportional to the container failure rate distribution:

$$e_{q,o}(n,t) = N \times I_q(n,t) \times c(t) \tag{E-15}$$

### Exposure Rate for Inner Inventories

The exposure rate for those inventories that are exposed instantaneously upon inner barrier failure is somewhat more complex:

$$e_{r,i}(n,t) = N \times I_r(n,t) \times g(t) \tag{E-16}$$

In this equation,  $g(t)$  represents the time-varying rate at which the inner inventory becomes “unprotected”. The inner inventory becomes “unprotected” when both the outer and the inner barriers have failed. Hence,  $g(t)$ , is a function of both the outer and inner barrier failure rates:

$$g(t) = \int_0^t [c(\tau) w(\tau, t) + c(\tau) w(t, \tau)] d\tau \tag{E-17}$$

The first term in the integral represents the contribution from those outer barriers that are failing at time  $t$  whose inner barrier had previously failed. The second

**Exposure Rate for Bound Inventories**

term represents the contribution from outer barriers that had failed prior to time  $t$  whose inner barrier is failing at time  $t$ .

The exposure rate for inventories that are exposed upon degradation of the matrix differs depending on whether degradation is described as being fractional or uniform (fractional rates are entered in units of inverse time, while uniform rates are entered in units of time).

Fractional Degradation Rate (and Congruent Dissolution)

Assuming fractional degradation rates (or solubility-controlled congruent dissolution of the matrix), the exposure rate for those inventories that are exposed upon degradation of the matrix is a function of the mass of species that is unprotected (i.e., outer and inner barriers have failed) but is still bound in an undegraded matrix, and the degradation rate of the matrix:

$$e_{s,b}(n,t) = N \times M_s(t) \times k_s(t) \times I_s(n,t) \tag{E-18}$$

$M_s(t)$  is the *fraction* of unprotected but undegraded matrix (and hence is unitless), and can be determined by solving the following differential equation:

$$\begin{aligned} dM_s(t)/dt &= (\text{rate at which matrix is being unprotected}) - (\text{rate at which unprotected matrix is being degraded}) \\ dM_s(t)/dt &= h(t) - M_s(t) \times k_s(t) \end{aligned} \tag{E-19}$$

The rate at which the matrix becomes unprotected,  $h(t)$ , differs depending on whether the matrix is within the outer barrier, within the inner barrier, or not within any barriers at all. If the matrix is within the outer barrier,  $h(t)$  is equal to  $c(t)$ ; if it is within the inner barrier,  $h(t)$  is equal to  $g(t)$ ; if it is not within any barrier at all,  $h(t)$  is equal to  $c(t)$ , which is computed as if all barriers have failed immediately at the start of the simulation.

If  $h(t)$  and  $k_s(t)$  are constant, the solution to Equation (E-19) is:

$$M_s(t) = \frac{h}{k_s} (1 - e^{-k_s t}) + M_s(0) e^{-k_s t} \tag{E-20}$$

Although  $h(t)$  and  $k_s(t)$  are functions of time, over a timestep, they are assumed to be constant. Hence, GoldSim numerically solves Equation (E-19) as follows:

$$M_s(t) = \frac{h(t - \Delta t)}{k_s(t - \Delta t)} [1 - e^{-k_s \Delta t}] + M_s(t - \Delta t) e^{-k_s \Delta t} \tag{E-21}$$

Uniform Degradation Rate

Assuming a uniform degradation rate over time  $T$ , the exposure rate for those inventories that are exposed upon degradation of the matrix is a convolution integral:

$$e_{s,b}(n,t) = N \int_0^t I_s(n,t) h(\tau \min\left(\frac{t-\tau}{T}, 1\right)) \delta\tau \tag{E-22}$$

If the matrix is within the outer barrier,  $h(t)$  is equal to  $c(t)$ ; if it is within the inner barrier,  $h(t)$  is equal to  $g(t)$ ; if it is not within any barrier at all,  $h(t)$  is equal to  $c(t)$ , which is computed as if all barriers have failed immediately at the start of the simulation.

**Algorithm for Congruent Dissolution of Waste Matrix**

The most advanced option for defining matrix degradation rates in the Source Inventories dialog is to assume that the matrix degrades based on solubility-limited dissolution.

To simulate this, GoldSim identifies the largest single species in the inventory, and treats this as the matrix material. Upon barrier failure, the matrix is then degraded at a rate that keeps the matrix species at its solubility limit within all Inventory Cells.

The algorithm that GoldSim uses to accomplish this is as follows:

- Once any barriers protecting the congruently-dissolved inventory fail, the Source element exposes the entire inventory, handing it off to the Inventory Cell or Cells (there may be more than one Inventory Cells, with each one receiving a specified fraction of the inventory).
- Each Inventory Cell then manages the dissolution process for its matrix material. Initially, all of the inventory will be shown by the Cell element as ‘precipitated mass’. As the simulation progresses, an increasing fraction of the matrix material will dissolve, and simultaneously the same fraction of the other species in the inventory will be separated from the matrix and made available for transport. These other species will then either dissolve or precipitate out, depending on their solubility limits.
- Note that the element’s ‘precipitated mass’ output reports the sum of the undissolved inventory that is still within the matrix plus any released inventory that has exceeded its solubility limit within the Cell.

During the solution process, GoldSim solves for the matrix degradation rate using an iterative approach:

1. At each time step, GoldSim first does a trial solution where an estimate is used for the rate at which the remaining undissolved matrix inventory is to be dissolved. At the end of this test solution, GoldSim evaluates the amount of precipitated matrix material remaining in the Cell, and adjusts the estimate and repeats the trial if necessary.
2. If there is any increase in precipitated matrix material, the step is repeated, but exposing only a portion of the remaining inventory such that the solubility limit will be exceeded by a small amount. This slight overshoot is intended to ensure that in the second iteration just enough of the matrix will be exposed to reach the solubility limit.
3. If the concentration of matrix material at the end of the time step falls below the solubility limit another trial solution is carried out using an increased matrix dissolution rate.

The iteration continues until an acceptable solution is found, which usually occurs within one or two trials. Once this happens the final solution for all nuclides is carried out for the step, using the matrix dissolution rate that was established during the trial.

GoldSim’s solution process for cell-networks solves each individual decay-family separately (a decay-family consists of one or more decay chains, combining decay-chains that have any chemical elements in common). The iterative solution process described above is only carried out for the decay-family that includes the waste matrix material. After it has found the current dissolution rate for the matrix then all of the decay-families are solved using that rate.

If the CT\_Module user option “Log cell-network details” is enabled then information regarding the dissolution rate and the iterative solution process is included in the model’s run log.

---

# Glossary of Terms

## **Advective Mass Flux Link**

A mass flux link in which a quantity of a medium is specified to flow from one pathway to another, carrying dissolved, sorbed, and/or suspended species with it.

## **Aquifer**

A transport pathway element that is intended to represent a feature that essentially behaves as a fluid conduit. An Aquifer pathway actually performs its computations by creating a temporary set of linked Cell elements during the simulation, which are subsequently removed at the end of the simulation.

## **Cell**

A transport pathway element that is mathematically equivalent to a finite difference node. Cells are commonly applied to simulate discrete compartments in an environmental system (such as ponds, lakes, shallow soil compartments, or the atmosphere).

## **Cell net**

A network of interconnected Cell pathways that are directly linked by coupled mass flux links.

## **Coupled Link**

A link between two elements which causes the elements to be solved in a coupled (rather than a sequential) manner. Coupled links can only be created when using an extension module.

## **Daughters**

Reaction products of a species. Species can decay into one or more daughters (or daughter products).

## **Diffusive Mass Flux Link**

A mass flux link in which species diffuse between pathways according to a concentration gradient.

## **Direct Transfer Mass Flux Link**

A mass flux link in which species are moved from one pathway to another based on a user-specified transfer rate.

## **Elements Array Label Set**

A special set of array labels that can only be populated and edited via the Species element. It consists of all of the chemical elements (or compounds) specified in the model. As such, it is smaller than or equal to the Species array label set.

## **External Pathway**

A transport pathway element that provides a mechanism by which external program modules for contaminant transport (e.g., analytical, finite element, or finite difference models) can be directly integrated into GoldSim.

---

## **Fluid**

An element in GoldSim for defining the properties of fluid media (such as water, air, or blood).

## **Fracture Network**

A complex network of one-dimensional conduits used by a Network Pathway to describe contaminant transport through fractured rock systems.

## **Fracture Set**

An element used in conjunction with a Network pathway that identifies the transport properties of each pipe in the pathway's fracture network.

## **Henry's Law constant**

The distribution ratio (i.e., partition coefficient) for a species between air and water. It is the ratio of a compound's abundance in the gas phase to that in the aqueous phase at equilibrium.

## **Impact Conversion Factors**

Species- and receptor-specific factors that convert concentrations in environmental media to impacts to receptors. They have dimensions of impact per unit concentration, and are vectors in GoldSim (by species).

## **Laplace Transform**

A method for solving certain types of differential equations that involves transforming the equations into an algebraic form that can be readily solved, and then using an inverse transform to retrieve the solutions of the original problem.

## **Mass Flux Link**

An interconnection between two transport pathways that defines the rate at which species move between the pathways.

## **Media**

Materials (such as water, sand, clay, air) that constitute (are contained within) transport pathways. GoldSim provides two types of elements for defining media: Fluids and Solids.

## **Network Pathway**

A transport pathway element that provides a computationally efficient way to simulate large, complex networks of one-dimensional conduits in order to describe contaminant transport through fractured rock systems.

## **Normal Link**

A standard link between two elements.

## **Partition Coefficients**

The ratio of the species' concentration in a medium to its concentration in the Reference Fluid at equilibrium. Partition coefficients are inputs to Solid and Fluid elements.

## **Pipe**

A transport pathway element that is intended to represent a feature that essentially behaves as a fluid conduit. Pipes are ideal for simulating processes

---

such as vertical transport through an unsaturated zone, and horizontal transport in aquifers, rivers, channels and pipes.

### **Precipitate Removal Mass Flux Link**

A mass flux link in which precipitated species are removed from one pathway to another based on a user-specified transfer rate.

### **Previous Value Link**

A mass flux link between two pathways in which the previous value (rather than the current value) of the output is referenced.

### **Receptor**

A group (usually of people) that could potentially receive impacts from contaminants in the environment. In GoldSim, a Receptor is an element that converts contaminant concentrations in the environment to impacts to a receptor group.

### **Reference Fluid**

A special type of Fluid element that provides a basis for defining partition coefficients between media for the various species in the model (i.e., the ratio of the species' concentration in the medium to its concentration in the Reference Fluid at equilibrium).

### **Solid**

An element in GoldSim for defining the properties of solid media (such as sand, clay and rock).

### **Source**

A point, line or area at which mass is added to a system. In GoldSim, a Source is a specialized element for introducing mass into a contaminant transport model, and is particularly useful when simulating mass emanating from gradually failing engineered barriers.

### **Species**

The chemical (or non-chemical, such as bacterial or viral) constituents that are stored and transported through an environmental system in a contaminant transport model. In GoldSim, the Species element defines all of the contaminant species being simulated (and their properties).

### **Species Array Label Set**

A special set of array labels that can only be populated and edited via the Species element.

### **Specific Activity**

A property of radioactive species, it defines the number of disintegrations per unit mass per unit time. It is typically defined in terms of Becquerels (Bq) or Curies (Ci) per gram (g). Bq and Ci both have dimensions of disintegrations per unit time.

### **Transport Pathway**

Physical components or compartments through which contaminant species can move and/or be stored, such as aquifers, lakes, sediments, surface soil and the atmosphere. GoldSim provides four different elements for simulating pathways.

---

## **Treatment Mass Flux Link**

A mass flux link in which species are filtered (treated) as they are moved from one pathway to another based on a user-specified fraction (treatment efficiency).

---

# Index

## A

Activating  
  Contaminant Transport Module 9

Adding  
  species 44

Advection  
  simulating 90

Advective mass flux links 90

  advecting particulates to/from  
    Aquifers 189

  advecting particulates to/from  
    External pathways 229

  advecting particulates to/from  
    Pipes 215

  advecting particulates to/from  
    Cells 138

  creating and editing 91

  directionality 95

  inputs and outputs 94

  sign convention 95

  to/from Aquifers 188

  to/from Cells 136

  to/from External pathways 228

  to/from Network pathways 244

  to/from Pipes 214

Advective velocity multiplier 79

Appendices, list of 6

Aquifer pathways 22, 174

  adding mass 179

  advection and diffusion of  
    particulates 189

  advective flux links 188

  area 178

  basic properties 177

  browser view 187

  comparison to Pipes 251

  computational details 189, 378

  computing concentrations 249,  
    373

  defined 22

  discrete changes 184

  dispersivity 178

  example model 176

  features 175

  fluid saturation 179

  geometry 178

  how they are calculated 189, 378

  infill medium 179

  initial/boundary conditions 179

  length 178

  modeling multi-dimensional  
    plumes 249, 373

  number of cells 179

  outputs 186

  retardation 177

  saving results 193

  simulating suspended solids 185

  source zone length 184

  transverse dispersion 249, 373

Area of Aquifer pathways 178

Area of Pipe pathways 198

Array labels  
  elements 57

  species 57

Associated Cells 268

  behavior 271

  defining 269

  inventory Cells 270

Atomic weight 54

Available porosities 77

## B

Bacteria 304

Barrier failure  
  by events 281

  controlling algorithm 280

  delaying and modifying 275

  distributions 277

  inner 276

  outer 273

Barrier failure distributions  
  exponential 279

  immediate 278

  table 280

  uniform 278

  user-defined 280

  Weibull 278

Barriers for Sources 271

  number of 264

  overview 272

Boundary condition  
  Aquifer pathways 179

  Cell pathways 126

  External pathways 224

  Network pathways 239

  Pipe pathways 200

## C

Cell nets 165

Cell pathways 119

  adding mass 126

  adding media 123

  advection of particulates 138

---

- advective flux links 136
- associated with a Source 268
- automatically generating 151
- basic properties 122
- browser view 135
- coupling to flow model 163
- coupling to Pools 163
- coupling to Reservoirs 163
- defined 21
- deleting media 123
- diffusion of particulates 141
- diffusive flux links 139
- direct transfer mass flux links 146
- discrete changes 132
- example model 120, 136, 144, 146, 148, 149, 162
- features 120
- flow balance 164
- initial/boundary conditions 126
- inventory Cells for a Source 270
- material balance considerations 164
- mathematical details 316
- outputs 133
- precipitate removal mass flux links 147
- saving results 173
- simulating solubility constraints 159
- simulating suspended solids 124
- solution algorithm 164
- solution precision 247
- treatment mass flux links 149
- understanding partitioning 125
- CellNet Generator
  - partially saturated media 157
- CellNet Generator 151
- Cloning
  - pathways elements 254
- Coating material for a Pipe 205
- Conditional Containers
  - placing pathways in 255
- Congruent dissolution of matrix 268
- Containers
  - Materials 42
- Contaminant Transport Module
  - activating 9
  - basic concepts 16
  - defining events 37
  - difference between RT and CT 4
  - learning to use 7
  - overview 13
  - representing variability 38
  - user requirements 5
  - what is 1

- Context-sensitive Help 10
- Conventions
  - to describe key combinations 9
  - to describe mouse actions 9
- Copying
  - pathway elements between models 255
  - pathways elements 254
  - Species and Media between models 85
- Coupled mass flux links 118
- CT and RT Module 4
- CT Module
  - building a model 26
  - changes to the user interface 25
- Cumulative input
  - Aquifer pathways 179
  - Cell pathways 126
  - External pathways 224
  - Network pathways 239
  - Pipe pathways 200
- D**
- Daughter products 52
- Decay
  - deactivating 58
  - defining rates for species 52
  - how GoldSim simulates 54
  - modeling complex reactions 299
  - spatial variability in rates 294
- Diffusion
  - simulating 95
  - through unsaturated porous media 142
- Diffusive fluxes tab 98
- Diffusive mass flux links 95
  - between different fluids 144
  - creating and editing 98
  - diffusing particulates to/from Cells 141
  - directionality 101
  - inputs and outputs 101
  - sign convention 101
  - specifying geometry 139
  - through unsaturated porous media 142
  - to/from Aquifers 188
  - to/from Cells 139
  - to/from Pipes 214
- Diffusive Reduction Formula for Fluids 70
- Diffusivity
  - particulate 79
  - reference 65, 70
  - relative 66, 70

- 
- Diffusivity Reduction Formula 65
    - for Reference Fluid 65
  - Direct transfer mass flux links 103
    - creating and editing 103
    - directionality 107
    - inputs and outputs 105
    - to/from Cells 146
  - Discrete changes
    - to a Cell pathway 132
    - to a Pipe pathway 204
    - to an Aquifer pathway 184
  - Dispersivity of Aquifer pathways 178
  - Dispersivity of Pipe pathways 199
  - DLLs for external pathways
    - running in a separate process 224
  - Doses 290
  - Dry density 75
- E**
- Effective time for barrier failure 275
  - Elements
    - array label set 57
  - Elements array label set 57
  - Email
    - support 11
  - Events in Contaminant Transport Module 37
  - Excessive transport rates 173
  - Exponential barrier failure
    - distribution 279
  - Exposure of contaminant mass 261
  - External pathways 219
    - adding mass 224
    - advection and diffusion of particulates 229
    - advective flux links 228
    - browser view 230
    - defined 24
    - details of implementing 385
    - example model 220
    - features 219
    - initial/boundary conditions 224
    - outputs 230
    - passing fluxes to/from 229
    - properties 222
    - saving results 231
    - specifying other inputs/outputs 226
- F**
- Failure
    - distributions for barriers 277
    - inner barrier for Sources 276
    - of packages by events 281
    - outer barrier for Sources 273
  - Fluid saturation for Aquifer pathways 179
  - Fluid saturation for Pipe pathways 199
  - Fluids 69
    - adding and editing 68
    - browser 82
    - copying between models 85
    - editing in Cells 123
    - inputs and outputs 82
    - modeling spatial variability 295
    - properties 69
    - saving results 74
  - Fraction of inflows mass flux links 112
  - Fractional degradation rate 266
  - Fracture networks
    - checking flow balance 238
    - creating and editing 235
    - explained 234
    - randomly sampling 241
    - sources and sinks 236
    - watch groups 237
  - Fracture sets 241
- G**
- GoldSim
    - blog 11
    - context-sensitive Help 10
    - Maintenance program 11
    - model library 11
    - online Help 10
    - training 11
- H**
- Hazard index 290
  - Heat transport 304
  - Help 10
  - Henry's Law constant 72
- I**
- ICRP database for decay rates 47
  - Immediate barrier failure
    - distribution 278
  - Impacts to Receptors 290
  - Infill medium for Aquifer pathways 179
  - Infill medium for Pipe pathways 199
  - Inflows

---

- creating and editing 91
- Initial condition
  - Aquifer pathways 179
  - Cell pathways 126
  - External pathways 224
  - Network pathways 239
  - Pipe pathways 200
- Inner barrier for Sources 276
- Inventories for Sources 265
  - congruent dissolution of matrix 268
  - matrix degradation rate 266
  - specifying 265
- Inventory Cells for a Source 270
- Isotopes
  - specifying 55
  - specifying media properties for 80

## K

- Key combinations
  - conventions to describe 9

## L

- Length of Aquifer pathways 178
- Length of Pipe pathways 198
- Looping Containers
  - placing CT/RT elements in 256

## M

- Maintenance program 11
- Manual
  - list of appendices 6
  - Notes in 9
  - organization of 5
  - Warnings in 9
- Mass flux links
  - advective 90
  - coupled 118
  - diffusive 95
  - direct transfer 103
  - fraction of inflows 112
  - integrating 253
  - normal 118
  - precipitate removal 107
  - previous value 118
  - treatment 112
- Mass input
  - to Aquifers 179, 184
  - to Cells 126
  - to External pathways 224
  - to Pipes 200, 204

- Mass input to Network pathways 239
- Material balance in Cell pathways 164
- Material balance in pathways 253
- Materials Container 42
- Matrix degradation rate 266
- Matrix diffusion
  - explained 206
  - specifying 208
- Media 64
  - copying between models 85
  - editing in Cells 123
  - introduction 29
  - modeling spatial variability 295
- Microorganisms 304
- Model library 11
- Models
  - building top-down 14
- Molecular weight 54
- Mouse actions
  - conventions to describe 9
- Moving
  - pathways elements 254

## N

- Network pathways 232
  - adding mass 239
  - advection and diffusion of particulates 245
  - advective flux links 244
  - browser view 243
  - controlling sources and sinks 239
  - defined 24
  - features 232
  - file format details 393
  - initial/boundary conditions 239
  - limitations 246
  - mass balance 246
  - mathematical details 383
  - outputs 243
  - properties 234
  - saving results 246
  - solution algorithm 246
- Normal mass flux links 118
- Number of cells in Aquifer pathways 179

## O

- Organization of manual 5
- Outer barrier for Sources 273
- Outflows
  - creating and editing 91

---

## P

- Packages for Sources 264
    - controlling discretization 280
    - failing by events 281
  - Particulates
    - advection to/from Cells 138
    - diffusion to/from Cells 141
    - diffusivity 79
    - in Aquifers 185
    - in Cells 124
    - in Pipes 212
  - Partition coefficients
    - for Solids 76
    - non-linear 297
    - specifying for isotopes 55, 80
    - use in Cells 125
    - use in Pipes 196
  - Partition Coefficients
    - for Fluids 71
  - Pathways 87, 90
    - Aquifers, defined 22
    - Cells, defined 21
    - comparing Pipes and Aquifers 89
    - copying between models 255
    - creating networks 89
    - defined 88
    - External, defined 24
    - in looping networks 256
    - integrating mass fluxes 253
    - introduction 31
    - introduction to connecting 33
    - material balance considerations 253
    - mathematical details 315
    - moving, copying, cloning 254
    - Network, defined 24
    - overview 17
    - overview of features 20
    - Pipes, defined 23
    - types 88
  - PBPK 308
  - Performance assessment 308
  - Perimeter of Pipe pathways 198
  - Physiologically-based
    - pharmacokinetic modeling 308
  - Pipe pathways 194
    - adding mass 200
    - advection and diffusion of particulates 215
    - advective flux links 214
    - area 198
    - basic properties 198
    - browser view 213
    - coating material 205
    - comparison to Aquifers 251
    - computing concentrations 249, 373
    - defined 23
    - discrete changes 204
    - dispersivity 199
    - example model 196, 207
    - features 195
    - fluid saturation 199
    - geometry 198
    - infill medium 199
    - initial/boundary conditions 200
    - length 198
    - limitations 217
    - mathematical details 347
    - matrix diffusion zones 206
    - modeling multi-dimensional plumes 249, 373
    - outputs 213
    - perimeter 198
    - retardation 197
    - saving results 217
    - simulating advection/dispersion 196
    - simulating suspended solids 212
    - solution algorithm 216
    - solution precision 247
    - source zone length 204
    - stagnant zones 209
    - storage zones 206
    - time-variable properties 215
    - transverse dispersion 249, 373
  - Plume function for Pipes and Aquifers 249, 373
  - Porosity 75
    - available 77
  - Precipitate removal mass flux links 107
    - creating and editing 108
    - directionality 112
    - inputs and outputs 110
    - to/from Cells 147
  - Previous value mass flux links 118
- ## R
- Radioactive species 55
  - Reactions
    - competing 303
    - modeling heat transport 304
    - modeling higher order 300
    - modeling stoichiometry 300
  - Receptors 289
    - browser view 292
    - defining 290
    - explained 290

---

- introduction 36
- overview 20
- saving results 292
- Reference Diffusivity
  - for Fluids 70
  - for Reference Fluid 65
- Reference fluid
  - changing rapidly 169
  - cloning 296
- Reference Fluid
  - browser 81
  - editing 64
  - inputs and outputs 81
  - properties 65
  - saving results 68
- Relative Diffusivities
  - for Fluids 70
  - for Reference Fluid 66
- Relative particulate diffusivity 79
- Retardation in Aquifers 177
- Retardation in Pipes 197
- RT and CT Module 4
- Run log
  - excessive transport rate 173
  - Inflow exceeds outflow 164
  - Reference Fluid volume changing rapidly 169
  - smallest substep failed 167
  - Zero Amount of Media in Cell 169

## **S**

- Safety assessment 308
- Solids 74
  - adding and editing 68
  - advanced properties 77
  - basic properties 75
  - browser 83
  - copying between models 85
  - editing in Cells 123
  - inputs and outputs 83
  - modeling spatial variability 295
  - saving results 80
- Solubilities
  - for Fluids 72
  - for Reference Fluid 67
  - simulating in Cells 159
  - solution algorithm for Cells 167
  - specifying for isotopes 55, 80
- Solution precision
  - CT Module 247
- Sorting species 46
- Source zone length
  - Aquifers 184
  - Pipes 204

- Sources 259
  - associated Cells 268
  - barrier failure 271
  - browser view 285
  - defined 260
  - defining 263
  - example model 283, 284
  - instantaneously moving mass 282
  - introduction 35
  - inventories 265
  - inventory Cells 270
  - mathematical details 399
  - outputs 282
  - overview 19
  - packages 264
  - processes modeled 261
  - saving results 286
  - when to use 261
- Sources and sinks for fracture networks 236
- Sources and sinks for Fracture networks
  - combining and splitting 239
- Species 43
  - adding 44
  - array label set 57
  - browser inputs 63
  - browser outputs 63
  - cloning 295
  - copying between models 85
  - decay rate database 47
  - editing 46
  - excluding 52
  - exporting to spreadsheet 58
  - ICRP database 47
  - importing from spreadsheet 58
  - including 52
  - introduction 27
  - isotopes 55
  - non-chemical constituents 303
  - properties 52
  - radioactive 55
  - removing 52
  - simulating heat 304
  - sorting 46
- Species array label set 57
- Spreadsheets
  - importing/exporting Species data 58
- Stagnant zones
  - explained 209
  - specifying 211
- Stoichiometry 54
  - complex 300
- Support
  - email 11

---

GoldSim user forum 11  
model library 11  
Suspended solids  
advection to/from Cells 138  
diffusion to/from Cells 141  
diffusivity 79  
in Aquifers 185  
in Cells 124  
in Pipes 212  
velocity multiplier 79

Weibull barrier failure distribution  
278

## T

Table barrier failure distribution  
280  
Technical support 11  
Top-down modeling 14  
Tortuosity 75  
Training course 11  
Transport Pathways 87  
Treatment mass flux links 112  
creating and editing 113  
directionality 118  
functionality 115  
inputs and outputs 116  
to/from Cells 149

## U

Uniform barrier failure distribution  
278  
Unsaturated diffusion 142  
User-defined barrier failure  
distribution 280

## V

Variability  
in decay rates 294  
in environmental systems 38  
in media properties 295  
representing 294  
Viruses 304

## W

Warning messages  
excessive transport rates 173  
Inflow exceeds outflow 164  
Reference fluid volume changing  
rapidly 169  
smallest substep failed 167  
Zero Amount of Media in Cell  
169  
Watch groups  
for fracture networks 237