

Sensitivity Analysis of Seals Permeability and Performance Assessment of Deep Borehole Disposal of Radioactive Waste

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Abstract: The concept of disposal of high-level radioactive waste in deep boreholes, and probabilistic performance assessment (PA) of a generic disposal system are described. A series of preliminary PA simulations, conducted to evaluate the possible migration of radionuclides to an accessible environment, are presented. The PA simulations provide estimates of radionuclide releases and mean annual radiation doses. The simulations utilized vertical fluxes from a thermal-hydrology process model. Of particular interest to the present study is an analysis of the sensitivity of borehole and surrounding rock permeability values. The analysis provides a bounding exercise of the performance of a generic deep borehole disposal system.

Keywords: Deep borehole disposal, thermal-hydrology, performance assessment, uncertainty analysis.

1. INTRODUCTION

The disposal of used nuclear fuel and high-level radioactive waste in deep boreholes is a feasible concept for long-term waste isolation [1-4]. The concept consists of drilling boreholes into crystalline rocks to a depth of 5 km, emplacing waste canisters in the lower 2 km, and sealing the upper 3 km. The viability of this disposal concept is supported by the presence of crystalline basement at many stable continental locations, and advances in drilling technology that permit reliable construction of deep boreholes at an acceptable cost. The safety of deep borehole disposal is supported by low permeability and high-salinity in deep crystalline rocks, limited interaction of deep fluids with shallower groundwater, and geochemically reducing conditions at depth, which limit the solubility and enhance the sorption of many radionuclides.

A potential pathway for the release of radionuclides to the biosphere is through the borehole seals or in the disturbed rock zone near the borehole. Thermally driven flow may transport radionuclides upward via this pathway. An analysis was carried out to assess the effectiveness of seals. The analysis consisted of a 3-D model of thermal-hydrologic flow in the borehole and surrounding rock, and a performance assessment model utilized to evaluate the potential for radionuclide migration. The performance assessment for a deep borehole disposal system or a geologic repository for radioactive waste is an analysis that provides estimates of the likelihood and magnitude of releases to the accessible environment and considers various scenarios [5-7]. The analysis starts with a preliminary consideration of a comprehensive list of potentially relevant features, events, and processes (FEPs) and the identification of those FEPs that appear to be most likely to affect long-term performance in deep boreholes [4]. Numerical simulations are performed based on the identified FEPs. The simulations described in this work do not include disruptive scenarios or borehole intrusion.

2. DEEP BOREHOLE THERMAL-HYDROLOGY MODEL

The deep borehole PA model uses vertical fluxes which are the output of the thermal-hydrology simulations. Numerical simulations of thermal-hydrology in the deep borehole disposal system were carried out with waste emplaced between 3000 m and 5000 m depth [2, 3]. The geometry of the system consisted of a disturbed zone of generally higher permeability than the host rock, within a cross-sectional area of 1 m² including the borehole, and low permeability host rock beyond the 1 m² cross-sectional area. For the simulations the seal material and the disturbed rock zone were represented with a single, combined, equivalent permeability and a total cross sectional area of 1 m². The combined material is termed disturbed

zone (DZ). The numerical grid uses a 3-D model domain with quarter symmetry boundary conditions, and consists of hexahedral elements with higher resolution near the boreholes. The simulations used the set-up of 9 boreholes with borehole spacing of 200 m (Figure 1). For the simulations the geothermal gradient was assumed to be 25°C/km, and the average near-surface temperature was assumed to be 10°C.

Thermal-hydrologic simulations were conducted for the disposal of a variety of high level nuclear waste types. However, for this work disposal of used commercial nuclear fuel (UNF) assemblies are only considered. The simulations were used to study temperature and fluid flow in the vicinity of the center borehole. Physical, thermal, and hydrologic properties representative of granite host rock at a depth of 4 km were used as shown in Table 1 [1]. Table 1 also shows permeability values for the host rock and the combined disturbed zone used for the base case. Bounding permeability values used in sensitivity analysis are given in Table 2, with an upper bounding case (rock permeability of 10^{-16} m^2 and DZ permeability of 10^{-12} m^2) representing a degraded seal system and a lower bounding case (rock permeability of 10^{-19} m^2 and DZ permeability of 10^{-19} m^2) representing a robust seal system.

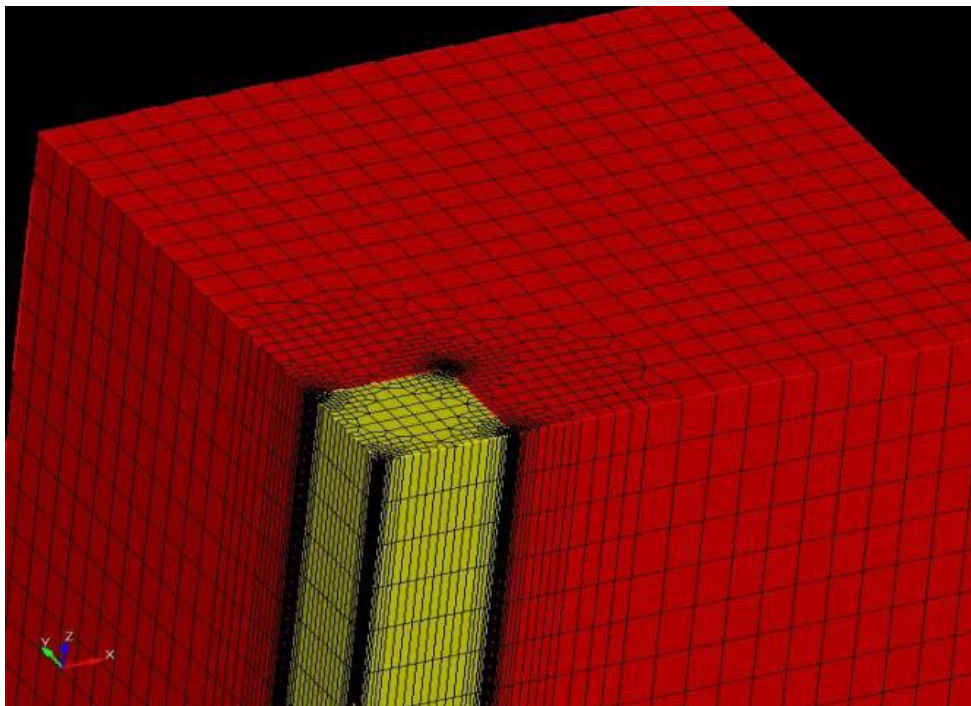


Figure 1. Mesh Used for Thermal-Hydrologic Simulations (Figure shows quarter symmetry for a system with 9 boreholes and 200-m borehole spacing)

Table 1. Parameter Values Used in Thermal-Hydrology modeling [1].

Parameter	Value
thermal conductivity (W/m °K)	3.0
density (kg/m ³)	2750.
porosity (-)	0.01
specific heat (J/kg °K)	790.
base case permeability of host rock (m ²)	1×10^{-19}
Base case permeability of borehole disturbed zone (m ²)	1×10^{-16}

Table 2: Rock and Disturbed Zone Permeability Values Used in Thermal-Hydrology Simulations

Host rock Permeability (m ²)	10 ⁻¹⁹	10 ⁻¹⁸	10 ⁻¹⁷	10 ⁻¹⁶
	Disturbed Zone Permeability (m ²)			
	10 ⁻¹⁵	10 ⁻¹⁴	10 ⁻¹³	10 ⁻¹²
	10 ⁻¹⁶	10 ⁻¹⁵	10 ⁻¹⁴	10 ⁻¹³
	10 ⁻¹⁷	10 ⁻¹⁶	10 ⁻¹⁵	10 ⁻¹⁴
	10 ⁻¹⁸	10 ⁻¹⁷	10 ⁻¹⁶	10 ⁻¹⁵
	10 ⁻¹⁹	10 ⁻¹⁸	10 ⁻¹⁷	10 ⁻¹⁶

For the analysis 400 disposal canisters were emplaced in the bottom 2 km of the borehole, followed by a series of robust sealing materials over 1 km length. The input includes decaying heat of UNF assemblies as a function of time. The input parameters of interest were disturbed zone (seal and disturbed rock zone) and host rock permeability values (Table 2). Thermal-hydrology simulations were conducted using the numerical code FEHM [8, 9] for a selected range of host rock and disturbed zone permeability values. The output of the simulations of interest was thermally driven vertical fluxes at different depths and times. Figure 2 shows a plot of vertical ground water flux versus time at 3000 m depth for the 20 permeability combinations given in Table 2. The plot line for the upper bounding case (rock permeability of 10⁻¹⁶ m² and DZ permeability of 10⁻¹² m²) is at the top, while the line for the lower bounding case (rock permeability of 10⁻¹⁹ m² and DZ permeability of 10⁻¹⁹ m²) is at the bottom, indicating that higher vertical fluxes are associated with higher permeability values. Between about 2000 years and 10,000 years the figure shows downward flow for cases with rock permeability of 10⁻¹⁹ m². The downward groundwater flow results from cooling and the corresponding thermal contraction of groundwater. For the degraded case, this effect is overcome by the broader pattern of upward thermal convection that occurs in the higher-permeability host rock and borehole. Figure 3 shows temperature versus time plots at 3000 m depth for the 20 permeability combinations. The temperature lines are nearly identical with a peak of about 50 °C rise, indicating that temperature is not very sensitive to rock and disturbed zone permeability values. This would indicate that the heat flow in the system is conduction dominated. This may be due to the fact that convection occurs mainly around the narrow borehole and excavated rock zone region, while conduction could occur in the larger intact rock.

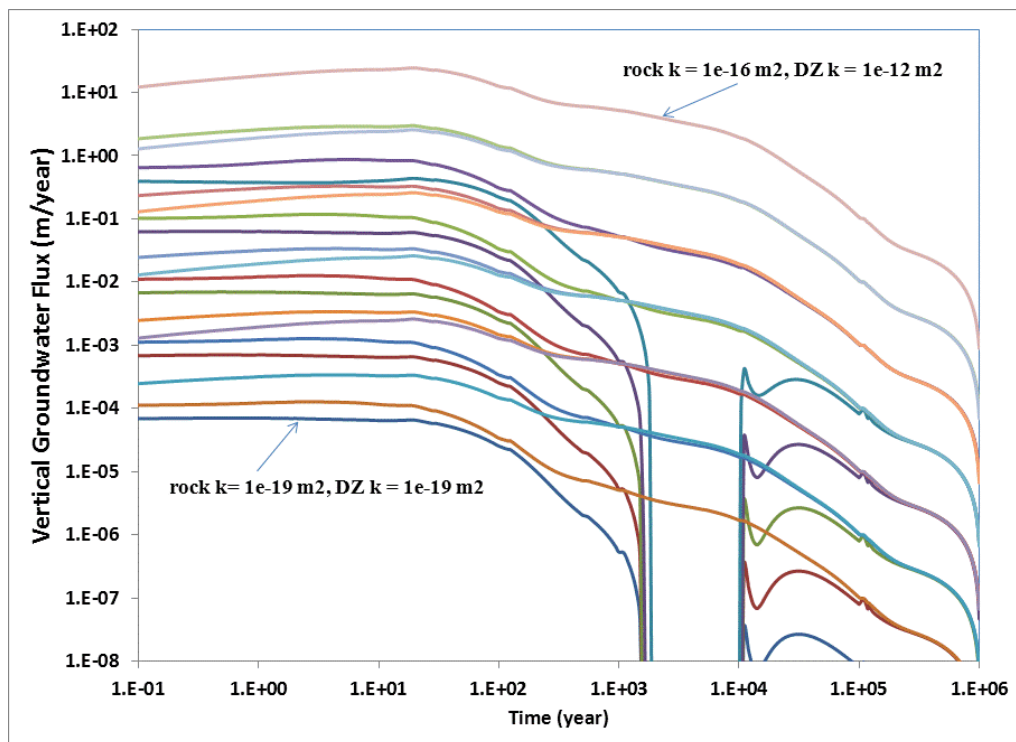


Figure 2. Vertical Groundwater Fluxes at Center of Corner Borehole at 3000 m Depth as a Function of Time for all Permeability Combinations Considered

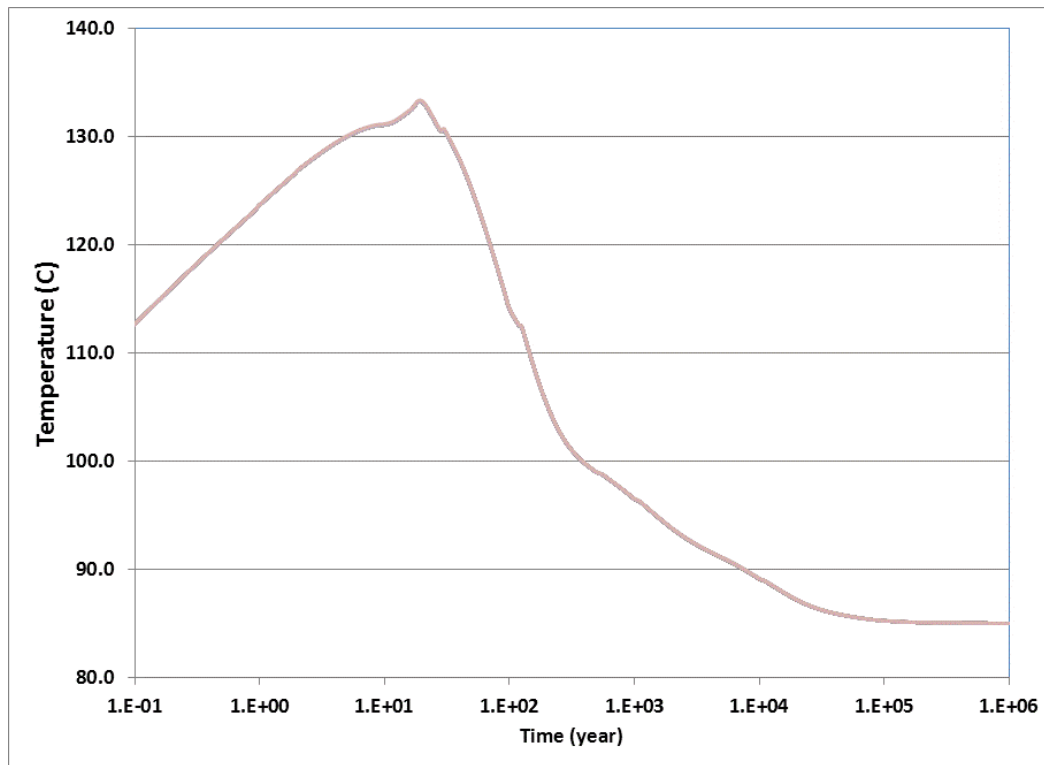


Figure 3. Temperature at Center of Corner Borehole at 3000 m Depth as a Function of Time for all Permeability Combinations Considered

3. DEEP BOREHOLE PERFORMANCE ASSESSMENT MODEL

The deep borehole PA model consists of three zones as shown in Figure 4 [4]:

- *Waste Disposal Zone* in the lower 2 km of the 5-km-deep borehole where the waste is emplaced.
- *Seal Zone* extending 1 km over the waste disposal zone, where robust sealing materials are placed.
- *Upper Borehole Zone* located in the top 2 km of the disposal borehole. In the deep borehole PA model, this zone is assumed to be connected to a surrounding aquifer. Any radionuclides that reach the top of the seal zone can enter an intersecting aquifer and be pumped and transported to the surface from a water supply well completed in the aquifer.

A series of probabilistic performance assessment simulations were then conducted using the thermally-driven vertical fluxes as input, to evaluate the possible migration of radionuclides to a “hypothetical” accessible environment. Radionuclide inventories and waste-form degradation rates representative of the selected waste type were included. For the disposal and seal zones vertical ground water fluxes from the thermal-hydrology simulations are used as input. For the upper borehole zone and the surrounding aquifer a constant groundwater flow rate of 0.00235 m³/year was used, representing a pumping well based on an analysis given in [1].

Radionuclide transport in the three deep borehole zones was simulated using the contaminant transport module of GoldSim [10, 11] to simulate radionuclide migration to the biosphere. Radionuclide transport processes simulated include advection, dispersion, diffusion, sorption, decay, and ingrowth. Flow and transport in the disposal and seal zones occur in the 1 m² cross-sectional area that consists of the borehole, seals, disturbed rock zone and grout. For this analysis radionuclides transported out of the seal zone are released into an aquifer where they are mixed and diluted. The radionuclides are then transported to the surface by a groundwater withdrawal well, and radiological doses are calculated. Radionuclide solubility calculations were based on the assumptions of reducing conditions in the disposal and seal zones, and less reducing conditions in the upper zone. Radionuclide sorption is simulated in all three zones.

Probability distributions were used to describe the uncertainty in parameter values for waste form degradation rate (i.e. dissolution rate), radionuclide solubility limits, and radionuclide sorption coefficients. Parameter values representative of the borehole disposal system and granite host rock were used for porosity, diffusion coefficient, effective dispersivity, bulk density, and waste package void volume. Waste form degradation was represented with an annual fractional degradation rate (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates for deep borehole disposal conditions [12]. Linear sorption coefficients for reducing conditions were used for radionuclide retardation [12]. Radionuclide solubility limits representative of geochemically reducing conditions in brine were applied in the disposal zone [12]. Solubility limits for the disposal and seal zones were based on assumed isothermal conditions of 100°C, representative of the average ambient temperature of deep granite, including uncertainty. For the upper zone linear sorption coefficients for less reducing conditions (as compared to the disposal and seal zones) are used to account for radionuclide retardation in that environment. Solubility limits for the upper zone were based on assumed isothermal conditions of 25°C. One of the simplifying assumptions taken in the PA simulations is that waste package failure occurs immediately after emplacement. This assumption would tend to over-estimate release.

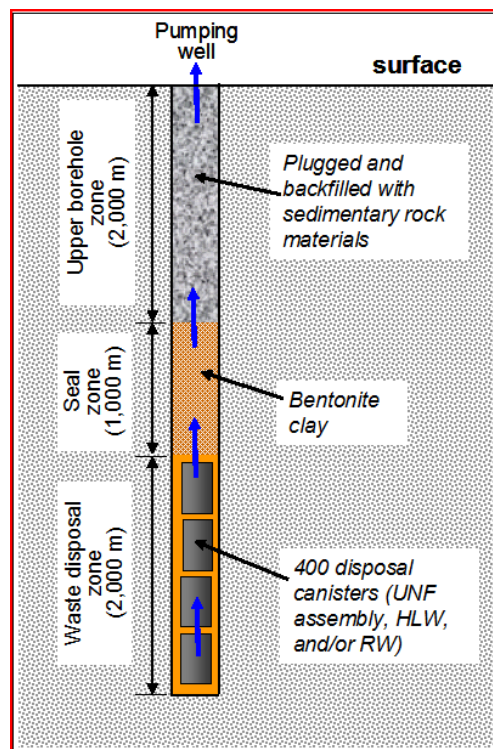


Figure 4. Schematic Illustration of Deep Borehole Disposal of Spent Nuclear Fuel Used in the Deep Borehole Model

4. PERFORMANCE ASSESSMENT SIMULATION RESULTS

Monte Carlo simulations were carried out for selected permeability cases for 100 realizations each. Latin Hypercube sampling was used for uncertain parameters with parameter distributions. The simulations were run to an assumed regulatory period of 1 million years. The deep borehole PA model provides estimates of radionuclide releases and mean annual radiation doses as output. Figure 5 shows estimated preliminary total dose rate as a function of time for selected permeability cases. The results provide an indication of the risk to human health associated with the range of representative values of permeability for the host rock and the disturbed zone. For the base case permeability values (rock permeability of 10^{-19} m^2 and DZ permeability of 10^{-16} m^2) radionuclide releases and dose rates at the surface are negligible. For the upper bounding permeability case (rock permeability of 10^{-16} m^2 and DZ permeability of 10^{-12} m^2) the simulated releases and

dose rates correspond to an acceptably small risk to human health. Figure 6 and 7 show mean dose rates of dominant radionuclides for the base and upper bound permeability cases. The simulations show that the non-sorbing radionuclides of Iodine (^{129}I) and Chlorine (^{36}Cl), and the mildly-sorbing radionuclide Technetium (^{99}Tc) account for most of the dose.

An analysis was also made to evaluate the impact of sorption and retardation on dose risk from the dominant dose contributor, ^{129}I . The radionuclide dominates the dose due to its unlimited solubility, no sorption or very weak sorption, and extremely long half-life (1.57×10^7 years). One approach to mitigate the potential release of ^{129}I is to load the seal materials with an effective sorbent for iodine. Simulations were conducted to evaluate potential impacts of iodine sorbent (getter) loaded in the seal zone on the deep borehole model performance. The simulations were performed for the upper bounding permeability case because it yields the higher peak mean doses (Figure 5). The impact was analysed with the use of a linear sorption (K_d) model for Iodine with a sorbent included in the seal material. The dose results for the upper bound permeability case with an Iodine getter are shown in Figures 5 and 7. The results indicate that use of proper Iodine sorbents could significantly reduce the peak dose.

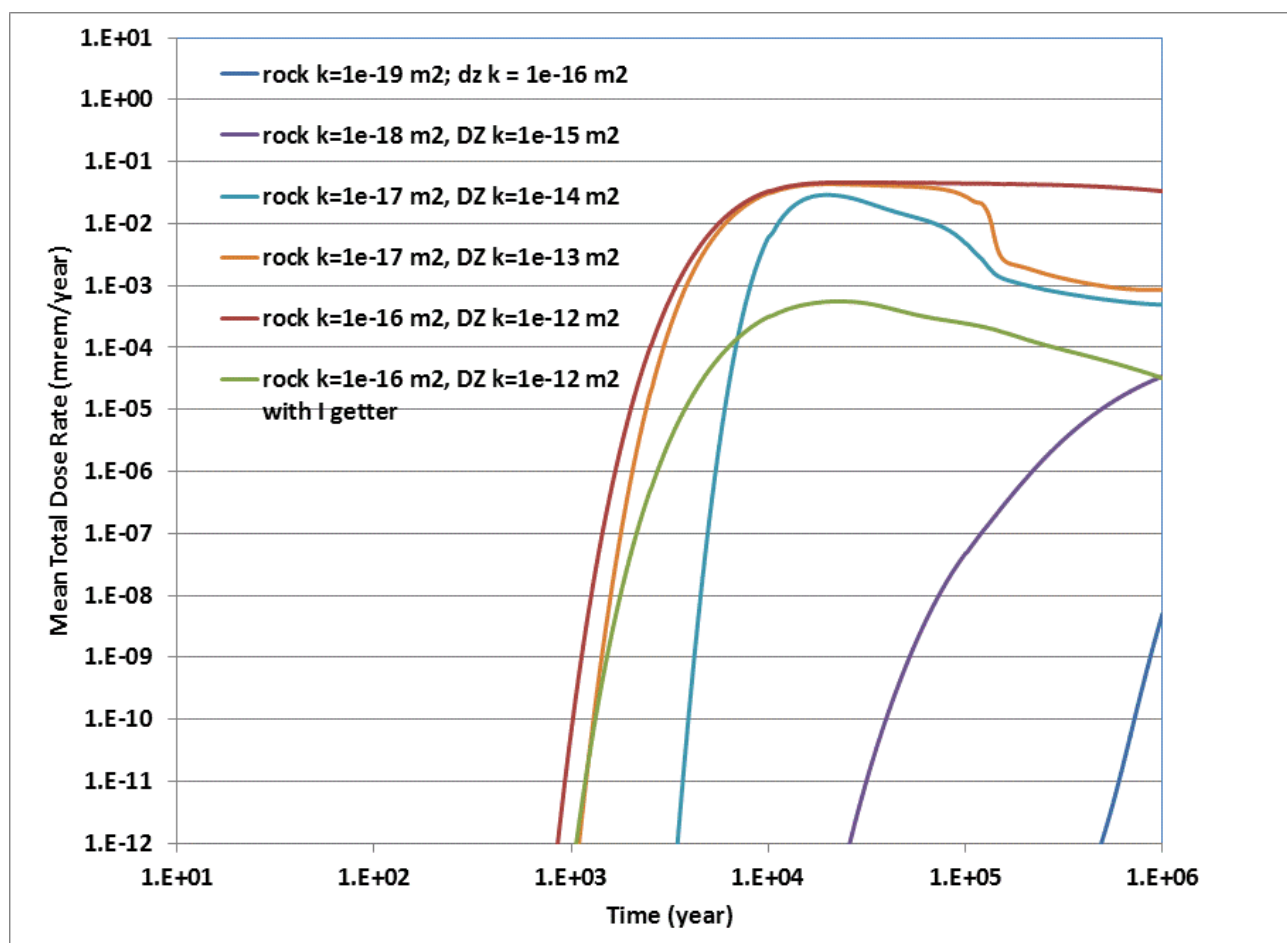


Figure 5. Simulated Total Dose Rate as a Function of Time from the Performance Assessment Model for Various Rock and Disturbed Zone Permeability Cases

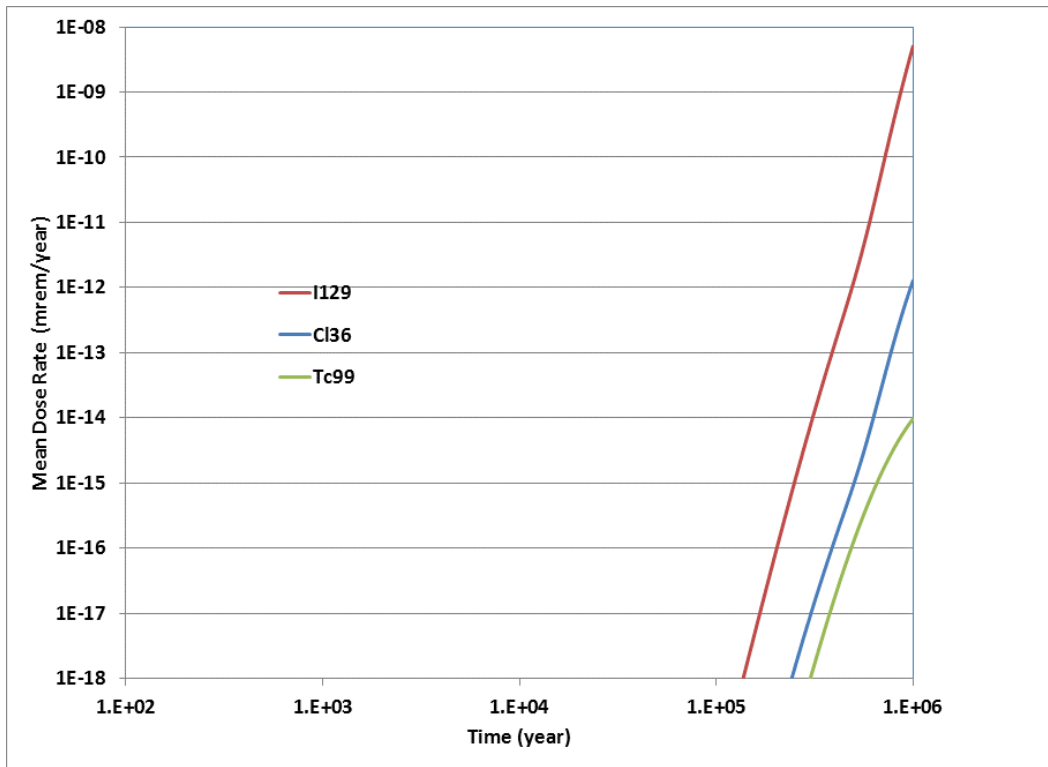


Figure 6. Simulated Mean Dose Rate as a Function of Time from the Performance Assessment Model for Dominant Radionuclides for the Base Case Rock and Disturbed Zone Permeability Values.

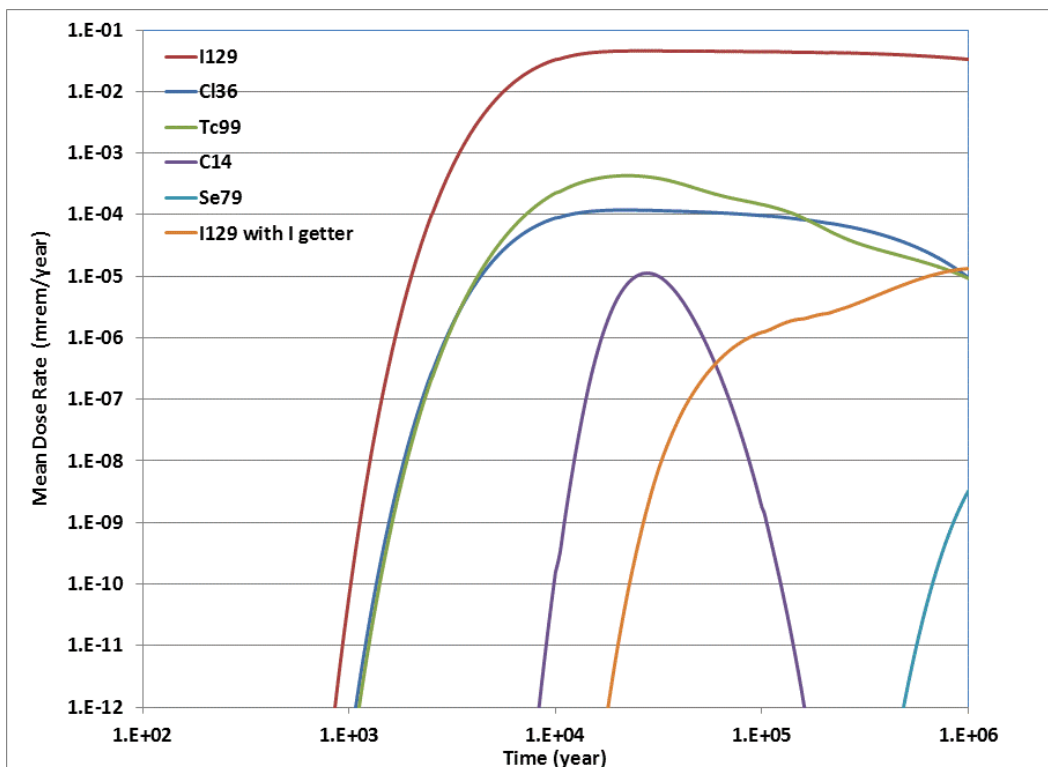


Figure 7. Simulated Mean Dose Rate as a Function of Time from the Performance Assessment Model for Dominant Radionuclides for the Upper Bounding Case Rock and Disturbed Zone Permeability Values. The Figure also Includes Iodine Mean Dose Rate for the Case with Iodine Getter.

5. SENSITIVITY ANALYSIS

A sensitivity analysis was also conducted to determine the contributions of individual uncertain input parameters to the total uncertainty, for each selected borehole and surrounding rock permeability combination given in Table 2. Sensitivity analysis, in this context, refers to the determination of the effects of epistemic uncertainty in sampled parameters. Partial rank correlation coefficients (PRCCs) were computed for total dose as a function of time. Furthermore a stepwise rank regression analysis was performed at 1 million years to confirm the results. The analysis also includes sensitivity to combined rock and disturbed zone permeability values, which were not part of the original sampled parameters.

Results from the scenarios (excluding the case with the use of iodine sorbent) presented in Section 4 have been assembled to include the effect of rock and disturbed zone permeabilities on total dose. For the purpose of illustration, we have considered that each of the scenarios were equally likely and associated an integer to each of them: 1 represents the base case (rock permeability of 10^{-19} m^2 and DZ permeability of 10^{-16} m^2). Numbers 2 to 5 have been associated to the four variations ordered by increasing permeability. As rock and disturbed zone permeability vary together, they have been associated with one common indicator function, PERMEA.

A Latin Hypercube Sampling (LHS) approach has been used to generate hundreds of values randomly selected from the discrete uniform distribution {1;2;3;4;5}. Each number was used to select the appropriate dose result from the corresponding scenario. With this approach (and considering that each scenario uses the same sample for other parameters), the LHS structure when incorporating this new variable (PERMEA) was preserved. Figure 8 displays PRCC over time for total dose. As expected, the indicator function over permeability (PERMEA) and the parameter for waste form degradation (WFDegRat) are the two most important parameters. Given the assumption made (all scenarios are equally likely) permeability plays a more important role. This is because vertical ground water flux is a strong function of rock and disturbed zone permeabilities (Figure 4). The results for waste form degradation are also consistent with what is expected as Iodine is the major contributor to the total dose (more than three orders of magnitude higher dose than the other radionuclides at 1 million years), and waste form degradation rate is the only uncertain input parameter that affects Iodine (Figure 7). Figure 8 also includes other less important parameters, which are sorption (Kd) input parameters for Technetium and Selenium in different zones (TcKdSZ, TcKdDZ, SeKdSZ, SeKdDZ).

A stepwise (rank) regression (SRR) analysis was also performed at the last time-step. The results, shown in Table 3, are consistent with the findings of the PRCC analysis (Figure 8) with permeability variation explaining about 88% of the variance, while waste form degradation rate explains 8% more.

Table 3: Stepwise Regression Analysis Over Total Dose at 1 Million Years, for Combined Results Including Effect of rock and DZ Permeabilities

Var. Name	R ²	R ² contribution	SRR
PERMEA	0.878	0.878	0.9656
WFDegRat	0.961	0.084	0.2905

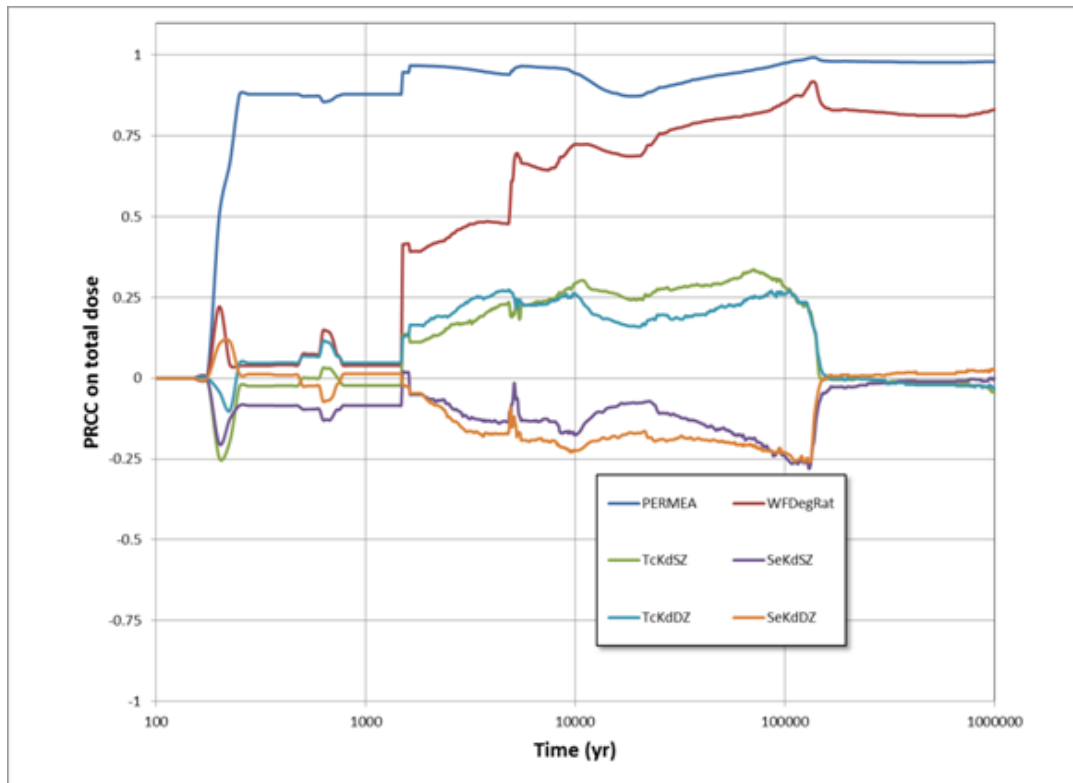


Figure 8. Partial Rank Correlation Coefficients on Total Dose Over Time for combined results including effect of rock and DZ permeabilities

6. CONCLUSION

A preliminary deep borehole PA model has been developed to evaluate aspects of the long-term performance of deep borehole disposal of high-level radioactive waste. A 3-D thermal-hydrology process model was used to provide thermally driven, vertical groundwater fluxes. The current model does not include disruptive scenarios or borehole intrusion. Simplifications have also been made such as the assumption of immediate waste package failure. Preliminary probabilistic simulations and a sensitivity analysis have been presented for UNF waste and bounding permeability cases.

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