SAND2012-1118C

Eleventh Probabilistic Safety Assessment and Management Conference (PSAM11) and the Annual European Safety and Reliability Conference (ESREL 2012) (June 25-29, 2012) Ref. 1751473

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

Teklu Hadgu, Bill Arnold, Joon Lee, Geoff Freeze, and Palmer Vaughn

Sandia National Laboratories, Albuquerque, New Mexico; USA 87185; thadgu@sandia.gov

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, performances 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, 2,3]. 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 drilling technology to construct 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 disposal to the accessible environment and considers various scenarios [4,5,6]. 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 [3]. 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 depth and the surface [2]. 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 m^2 around the borehole, and low permeability host rock beyond the 1-m^2 cross-sectional area. For the simulations the seal material and the disturbed zone were represented with a single, combined, equivalent permeability and a total cross sectional area of 1 m^2. 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. For the simulations the set-up of 9 boreholes with borehole spacing of 200 m was used (Figure 1). For the simulation, 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. For this work disposal of used commercial used nuclear fuel (UNF) assemblies are 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.

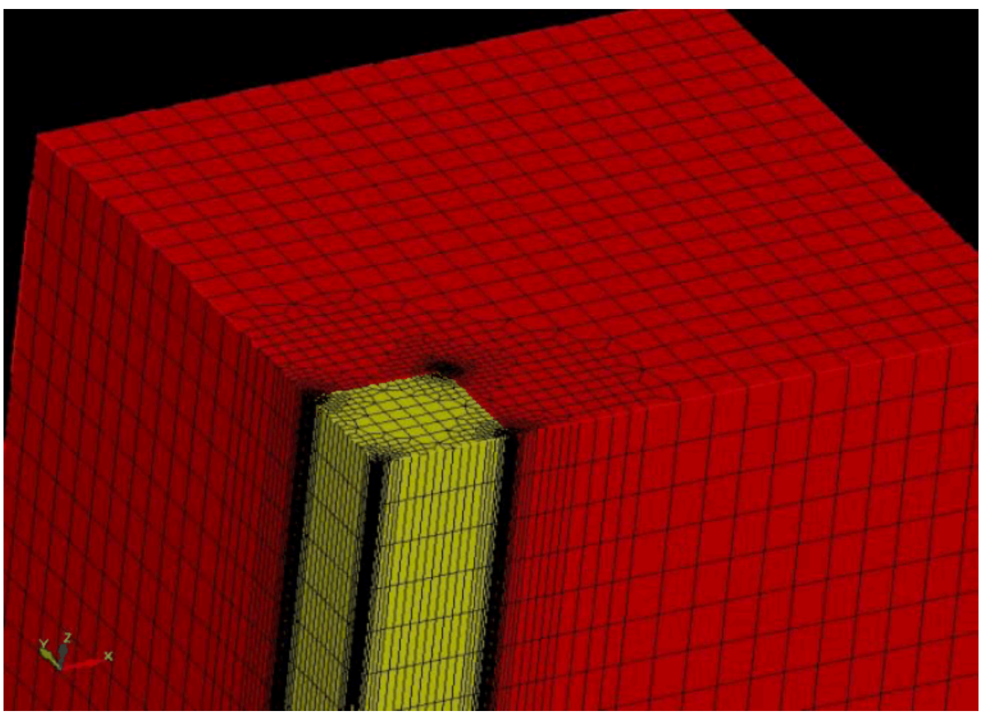


Figure 1. Mesh Used for Thermal-Hydrologic Simulations (Figure shows quarter symmetry for a system with 9 boreholes and 200-m borehole spacing)

Table 1. Parameter values used in thermal-hydrology modeling.

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 x 10^{-19}
Base case permeability of borehole disturbed zone (m^2)	1 x 10^{-16}

Table 2: Rock and disturbed zone (including seals) permeability values used in FEHM 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 [7, 8] for a selected range of host rock and disturbed zone permeability values. The output of the simulations 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 line for the upper bounding case (rock permeability of 10^{-16} m^2 and DZ permeability of 10^{-12} m^2) is at the top, while the line for the lower bounding case (rock permeability of 10^{-19} m^2 and DZ permeability of 10^{-19} m^2) 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} m^2. 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 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.

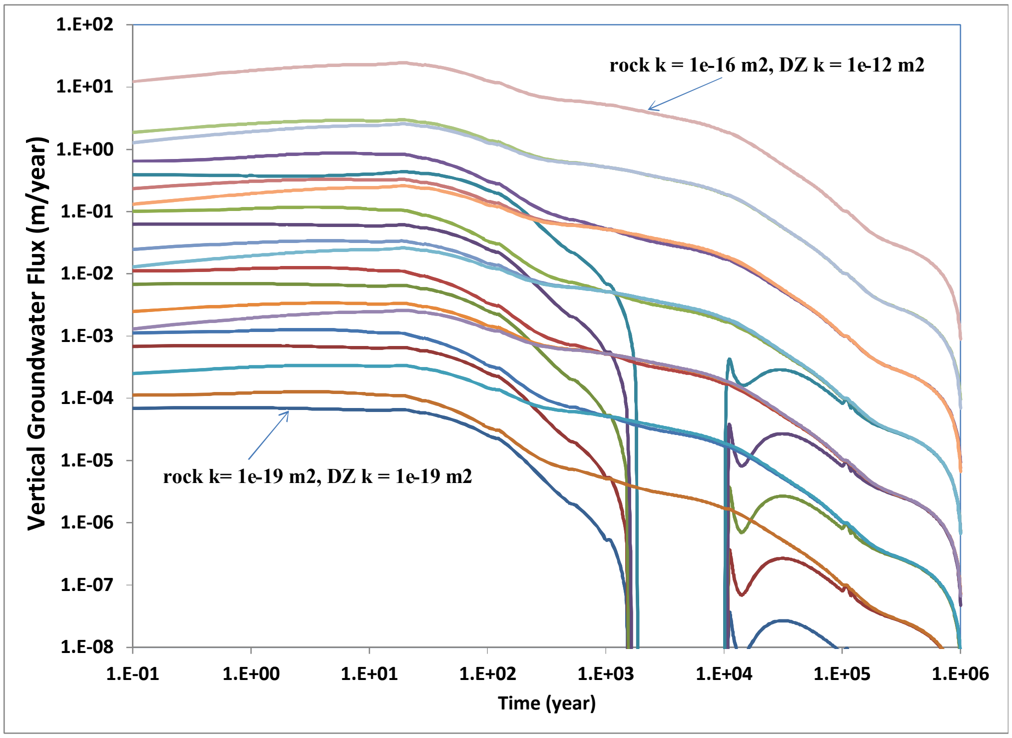


Figure 2: Vertical groundwater fluxes at center of corner borehole at 3000 m depth as a function of time for all permeability combinations considered

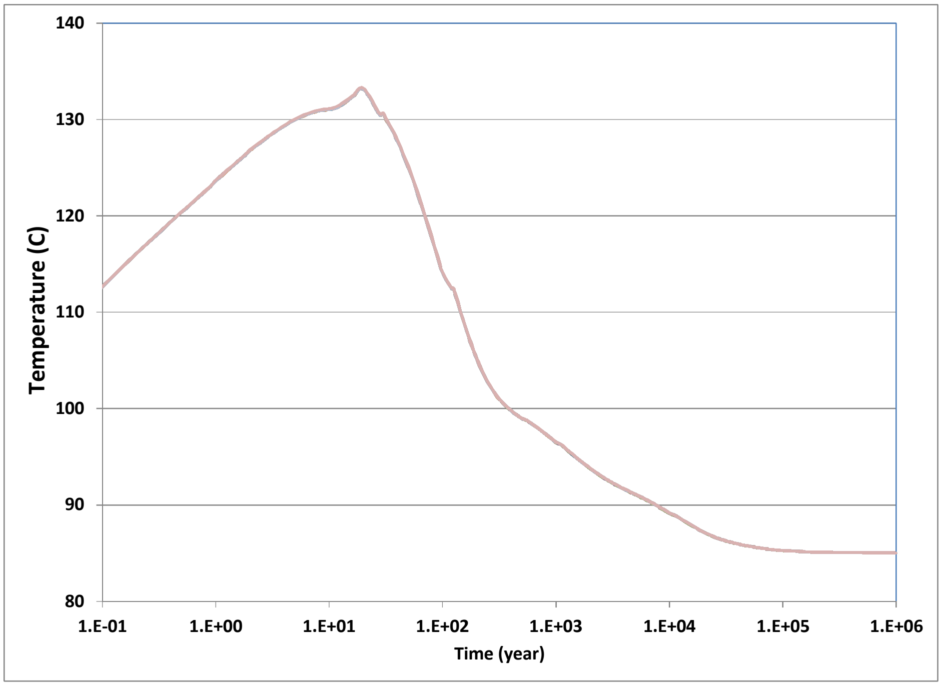


Figure 3: Temperature at center of corner borehole at 3000 m depth as a function of time for all permeability combinations considered

3. DEEP BOREHOLE PERFORMANCE ASSESSMENT MODEL

The deep borehole PA model consists of three zones as shown in Figure 4 [3]:

- *Waste Disposal Zone* 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.

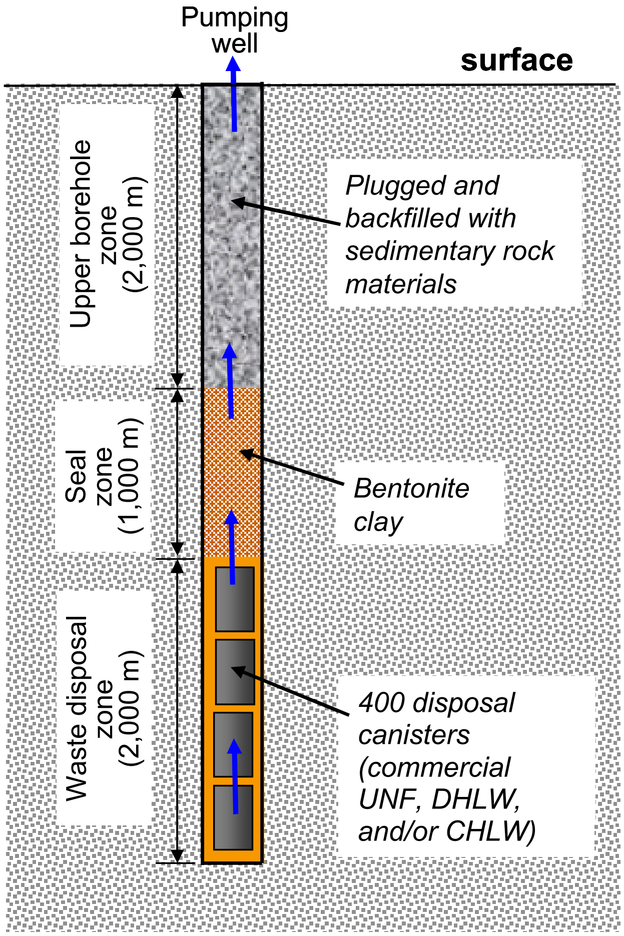


Figure 4. Schematic Illustration of Deep Borehole Disposal of Spent Nuclear Fuel Used in the Deep Borehole Model

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 m^3/yr was used, representing a pumping well based on an analysis in [1].

Radionuclide transport in the three deep borehole zones was modeled using the contaminant transport module of GoldSim [9, 10] to simulate radionuclide migration to the biosphere. Radionuclide transport processes modeled include advection, dispersion, diffusion, sorption, decay, and ingrowth. Flow and transport in the disposal and seal zones occur in 1 m^2 cross-sectional area that consist 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 modeled in all three zones.

Probability distributions were used to describe the uncertainty in parameter values for waste form degradation 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. Linear sorption coefficients for reducing conditions were used for radionuclide retardation [11]. Radionuclide solubility limits representative of geochemically reducing conditions in brine were applied [11] in the disposal zone. 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.

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 10^6 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 values (rock permeability of 10^{-19} m^2 and DZ permeability of 10^{-16} m^2) radionuclide realizes 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 shows the corresponding mean dose rates of dominant radionuclides. 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 x 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 analyzed with the use of a linear sorption (Kd) model for iodine for a bentonite seal material. The dose results for the upper bound permeability case with an iodine getter are shown in Figure 5. The results indicate that use of proper iodine sorbent could significantly reduce the peak dose.

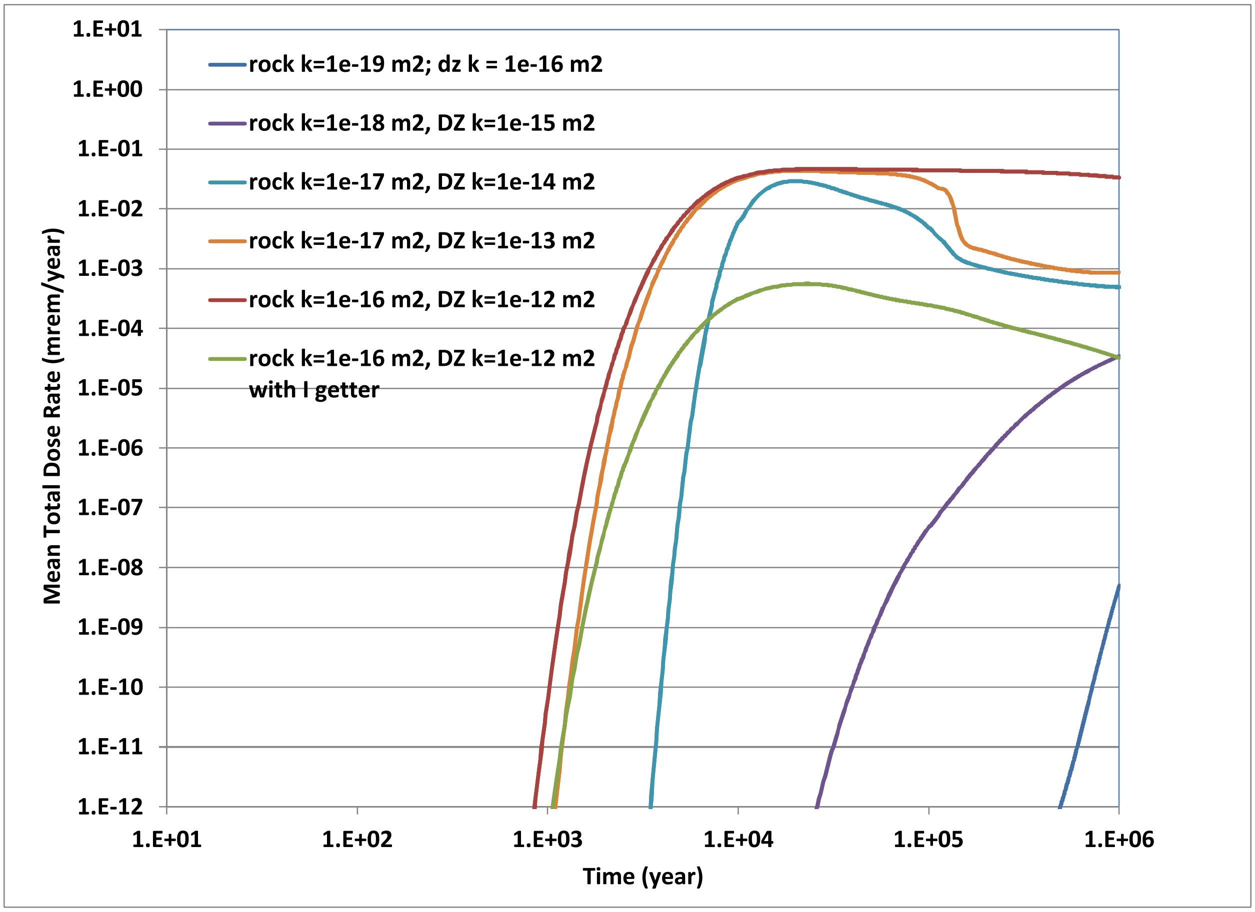


Figure 5. Simulated total dose rate as a function of time from the performance assessment model for various rock and disturbed zone permeability cases.

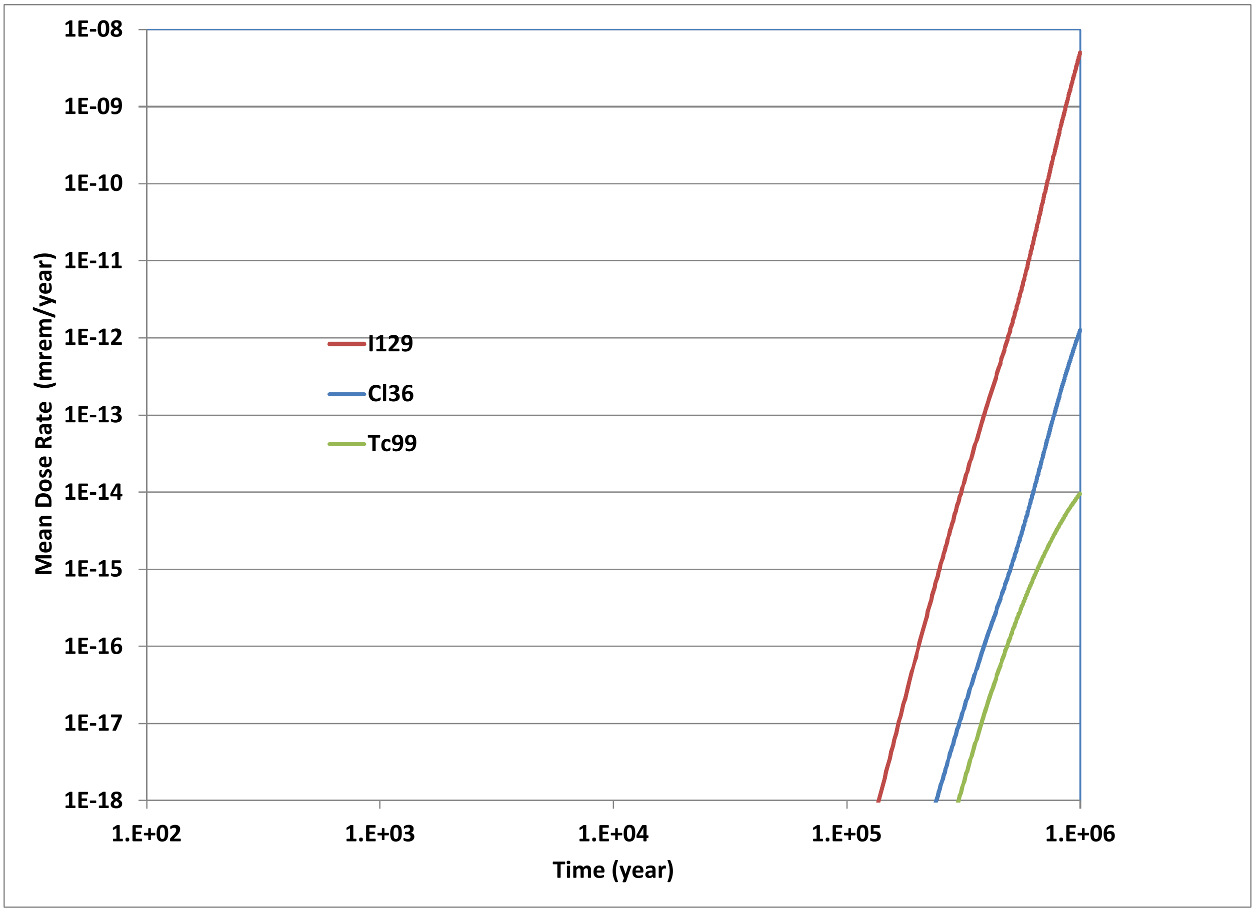
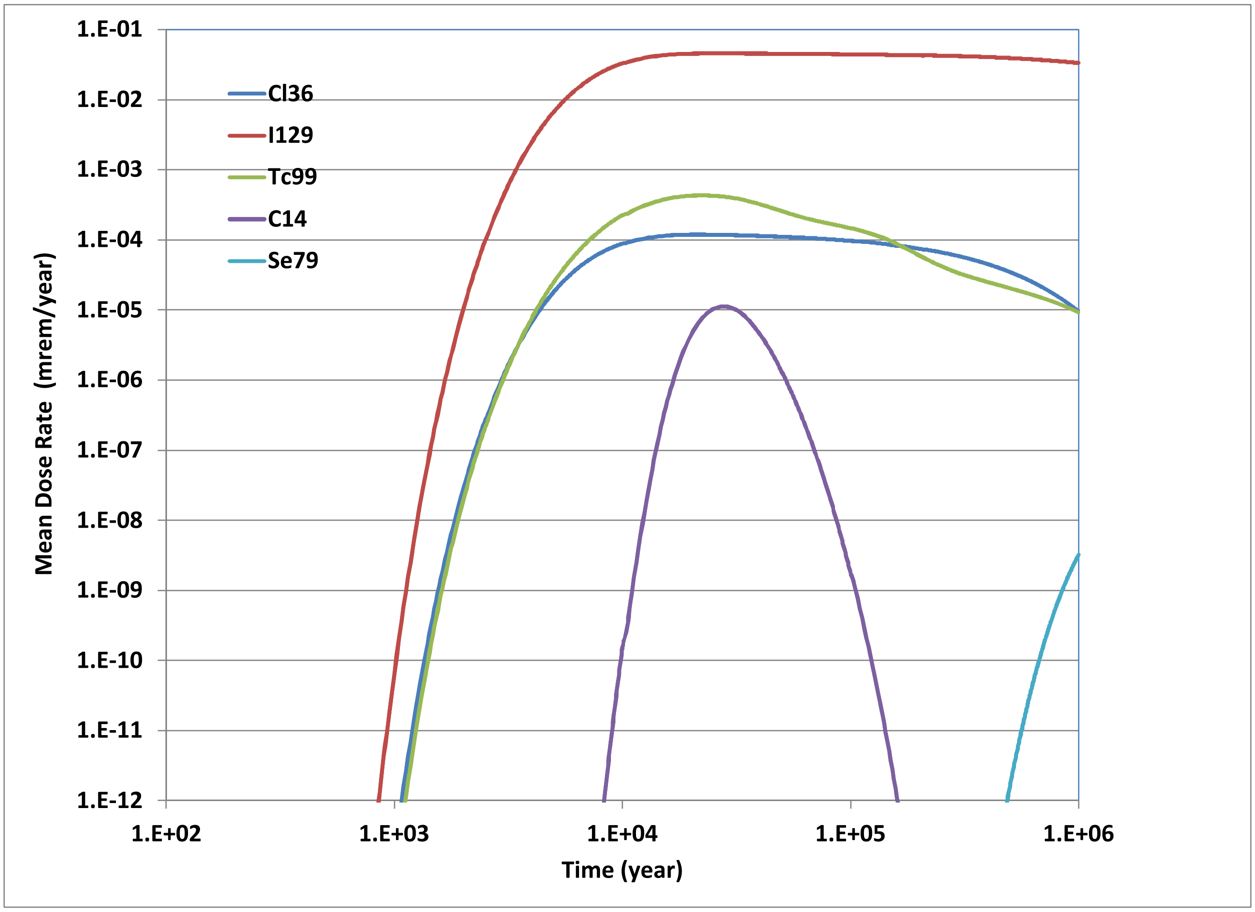


Figure 6. Simulated mean dose rate as a function of time from the performance assessment model for dominant radionuclides for the base case rock and disturbed zone permeability values.



5. CONCLUSIONS

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 have been made for UNF waste and bounding permeability cases.

Acknowledgments: Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. The views expressed in this article are those of the authors and do not necessarily reflect the views or policies of the department of energy or Sandia National Laboratories.

References

[1] Brady, P.V., B.W. Arnold, G.A. Freeze, P.N. Swift, S.J. Bauer, J.L. Kanney, R.P. Rechard, and J.S. Stein. *Deep Borehole Disposal of High-Level Radioactive Waste*. 2009. SAND2009-4401. Albuquerque, NM: Sandia National Laboratories.

[2] Arnold, B.W., T. Hadgu, D. Clayton, and C. Herrick. Thermal-hydrologic-Chemical-Mechanical Modeling of Deep Borehole Disposal. *2011 International High-Level Radioactive Waste Management Conference, April 10-14, 2011*, Albuquerque, NM.

[3] Swift, P.N., B.W. Arnold, P.V. Brady, G. Freeze, T. Hadgu, J. Lee, and Y. Wang. "Preliminary Performance Assessment for Deep Borehole Disposal of High-Level Radioactive Waste." *2011 International High-Level Radioactive Waste Management Conference, April 10-14, 2011*, Albuquerque, NM.

[4] Helton JC et al. *Characterization of Stochastic Uncertainty in the 1996 Performance Assessment for the Waste Isolation Pilot Plant.* Reliability Engineering and System Safety: 2000,69(1-3),167-189.

[5] Helton JC et al. *Characterization of Subjective Uncertainty in the 1996 Performance Assessment for the Waste Isolation Pilot Plant.* Reliability Engineering and System Safety:2000,69(1-3),191-204.

[6] SNL (Sandia National Laboratories). *Total System Performance Assessment Model/Analysis for the License Application.*MDL-WIS-PA-000005 Rev 00, AD 01.Las Vegas, NV: U.S. Department of Energy Office of Civilian Radioactive Waste Management, 2008.

[7] Zyvoloski, G.A. *FEHM: A control volume finite element code for simulating subsurface multiphase multi-fluid heat and mass transfer*. 2007. Los Alamos Unclassified Report LA-UR-07-3359. Los Alamos, NM: Los Alamos National Laboratory.

[8] Zyvoloski, G.A., B.A. Robinson, Z.V. Dash, and L.L. Trease. *Summary of the models and methods for the FEHM application A Finite-Element Heat- and Mass-Transfer Code*. 1997. LA-13307-MS. Los Alamos, NM: Los Alamos National Laboratory.

[9] GoldSim Technology Group. *GoldSim Probabilistic Simulation Environment User's Guide, Version 10.5. Volumes 1 and 2*. 2010. Issaquah, Washington: GoldSim Technology Group LLC.

[10] GoldSim Technology Group. *GoldSim version 10.50*. 2011.

[11] D. Clayton, G. Freeze, T. Hadgu, E. Hardin, J. Lee, J. Prouty, R. Rogers, W. M. Nutt, J. Birkholzer, H.H. Liu, L. Zheng, S. Chu: Generic Disposal System Modeling Fiscal Year 2011 Progress Report, Fuel Cycle Research and Development, Used Fuel Disposition, USDOE (SAND2011-5828P). 2011.