A Prototype Performance Assessment Model for Generic Deep Borehole Repository for High-Level Nuclear Waste – 12132

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ABSTRACT

A deep borehole repository is one of the four geologic disposal system options currently under study by the U.S. DOE to support the development of a long-term strategy for geologic disposal of commercial used nuclear fuel (UNF) and high-level radioactive waste (HLW). The immediate goal of the generic deep borehole repository study is to develop the necessary modeling tools to evaluate and improve the understanding of the repository system response and processes relevant to long-term disposal of UNF and HLW in a deep borehole. A prototype performance assessment model for a generic deep borehole repository has been developed using the approach for a mined geological repository. The preliminary results from the simplified deep borehole generic repository performance assessment indicate that soluble, non-sorbing (or weakly sorbing) fission product radionuclides, such as I-129, Se-79 and Cl-36, are the likely major dose contributors, and that the annual radiation doses to hypothetical future humans associated with those releases may be extremely small. While much work needs to be done to validate the model assumptions and parameters, these preliminary results highlight the importance of a robust seal design in assuring long-term isolation, and suggest that deep boreholes may be a viable alternative to mined repositories for disposal of both HLW and UNF.

INTRODUCTION

The U.S. is currently re-evaluating the policy on commercial used nuclear fuel (UNF) and high-level radioactive waste (HLW) management. As part of the Fuel Cycle Research and Development (FCRD) program supported by the U.S. DOE Office of Nuclear Energy, the Used Fuel Disposition (UFD) campaign has been studying generic disposal system environment (GDSE) concepts to support the development of a long-term strategy for geologic disposal of commercial UNF and HLW. The GDSE study focuses on the comparative analysis of different generic disposal system (GDS) options, and a deep borehole repository is one of the options currently under study. The immediate goal of the deep borehole GDS study is to develop the necessary modeling tools to evaluate and improve the understanding of the repository system response and processes relevant to long-term disposal of high-level nuclear waste in deep boreholes.

Deep boreholes have been proposed for many decades as an option for permanent disposal of high-level nuclear waste. Figure 1 shows a schematic illustration of deep borehole disposal of UNF and HLW [1, 2]. This disposal concept is straightforward, and generally calls for drilling boreholes to a depth of approximately 5,000 m into crystalline basement rocks. Waste is placed in the lower 2,000 m of the hole, and the upper remaining portion (3,000 m) of the hole is sealed to provide effective isolation from the biosphere. Multiple boreholes could be constructed at a single disposal site, with the spacing between boreholes chosen based on thermal considerations [3-5]. The conceptual description of the borehole design, its basis and the operations of the system are described in Refs. [1-3]. Other borehole disposal concepts have been proposed, including the construction of multiple emplacement boreholes drilled at an angle from a single vertical hole [6], and the example analyzed in this paper is simply one of many possible configurations. The potential for excellent long-term performance has been recognized in many previous studies (refer to the references cited in Ref. [1]).

This paper presents a prototype performance assessment model for a deep borehole GDS, which was developed using the same performance assessment methodology applied to mined geologic repositories for high-level nuclear waste [1, 2]. The paper also discusses the preliminary analysis results, emphasizing key attributes of a deep borehole GDS that are potentially important to the long-term safe disposal of nuclear waste.

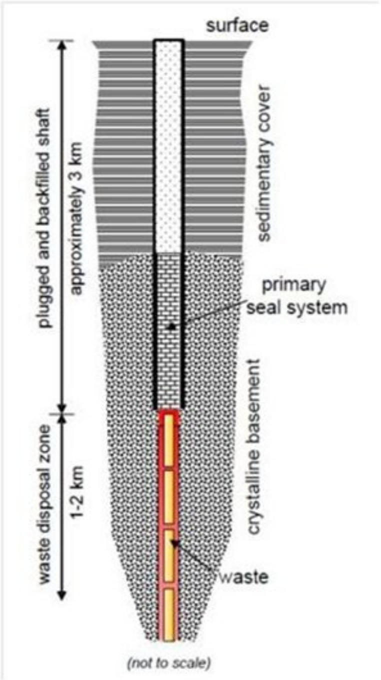

Figure 1. Schematic illustration of deep borehole disposal of UNF and HLW [1].

CONCEPTUAL MODEL

Based on the conceptual design described above, the conceptual model for radionuclide release and transport from a deep borehole GDS was developed for a simplified and conservative representation of the release scenarios identified following preliminary FEP screening as described in Ref. [2]. Figure 2 shows a schematic for the conceptual model. The deep borehole at a total depth of 5,000 m is divided into three zones: the bottom 2,000 m for waste disposal (referred to as the “disposal zone”), the next 1,000 m sealed with compacted bentonite clay (referred to as the “seal zone”), and the top 2,000 m plugged and backfilled with sedimentary rock materials (referred to as the “upper zone”). For simplification, a uniform cross sectional area of 1 m^2, representing the borehole, its content, and the surrounding disturbed rock zone, is assumed for the entire length of borehole.

It is assumed that a disposal canister with a length of about 5 m is used to lower the waste to the disposal zone, and that the canisters are stacked vertically in the disposal zone. Each canister contains a commercial UNF assembly, a DOE HLW canister, or a reprocessing HLW canister. The borehole disposal interval of 2,000 m would allow for emplacement of approximately 400 waste disposal canisters in a single borehole. The initial waste inventory is uniformly distributed over the length of the disposal zone. The radionuclide inventory per disposal canister for each waste type is provided in Ref. [7].

In the simplified performance assessment model, the disposal zone is assumed at a constant ambient temperature of 100°C. The model ignores the relatively short-lived transient higher temperatures in the borehole following waste disposal [2]. The seal and upper zones are assumed at a constant temperature of 25°C. The radio-elemental solubility constraints for chemically reducing brines at 100°C are applied to the disposal zone (Ref. [8] for the solubility constraints of key radionuclides at 100°C and Ref. [7] for other radionuclides); the solubility constraints for less reducing or slightly oxidizing brines at 25°C are applied to the seal and upper zones (Ref. [8] for the solubility constraints of key radionuclides at 25°C and Ref. [7] for other radionuclides).

No disposal canister performance is considered in the current model, and the canister is assumed to fail at the time of borehole closure. The annual fractional degradation rate models are used to model radionuclide release from the waste form (e.g., commercial UNF and HLW glass). The possible rapid release of a gap fraction of mobile radionuclides in the waste form is not included in the current model.

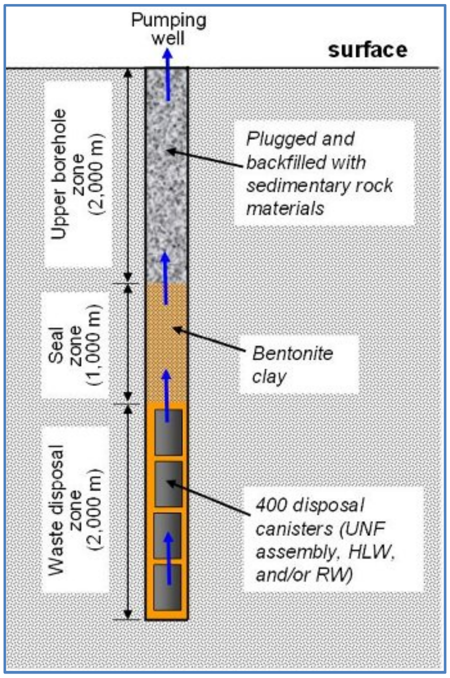

Figure 2. A Schematic illustrating the conceptual model for performance assessment of generic deep borehole disposal.

In the deep borehole GDS model, vertical water flow in the borehole is driven by thermal hydrology as a result of decaying heat from the radioactive waste. Thermally driven hydrologic flow within the waste disposal zone and seal zone and surrounding fractured rock annulus is calculated using a nine-well array (200 m spacing between holes) in a three-dimensional flow model [4] implemented in the FEHM software code [9]. Flow rates vary as a function of time and depth.

The model simulates radionuclide transport in a single borehole (the center borehole in the array used in the thermal hydrology model). Modeled processes include advection, dispersion, diffusion, sorption, and radionuclide decay and in-growth. Sorption coefficients in all three zones are given in Ref. [7].

The model assumes that water is pumped continuously to the surface from an aquifer intersecting the deep borehole at a depth of 2,000 m with a withdrawal well assumed to be located directly above the deep borehole. A constant volumetric groundwater rate of 2.35×10^{-3} m^3/year is used in the upper zone for the entire simulation period. The rate was obtained from an analysis to match the breakthrough curve (of pumping well for 1000 people) in Ref. [2] using the one-dimensional transport model.

The model assumes a "hypothetical" biosphere at the groundwater pumping location, and the International Atomic Energy Agency's (IAEA) BIOMASS Example Reference Biosphere 1B (ERB 1B) dose model [10] is used to convert the dissolved radionuclide concentrations in groundwater to an estimate of annual dose to a receptor based on drinking well water consumption. The model assumes that radionuclide releases are contained in groundwater extracted at a rate of 1×10^4 m^3/year in the aquifer and an individual water consumption rate of 1.2 m^3/year [10].

Note that applying the biosphere model at the hypothetical groundwater pumping location is an arbitrary modeling choice to produce a uniform performance measure for comparative studies of a deep borehole GDS and does not indicate any realistic dose implications. Therefore, the results presented in this paper *should not* be construed as being indicative of the true performance of a deep borehole GDS or compared to any regulatory performance objectives regarding repository performance.

MODEL IMPLEMENTATION AND STRUCTURE

Goldsim software [11] was used as the framework for model implementation and simulations. Figure 3 shows the Goldsim model structure of the deep borehole GDS model, and the model components for radionuclide transport in the borehole. The model components are given specific names indicative of their function in the overall model. The source-term model (see Ref. [6] for detailed discussions) is implemented in the following model components: *Materials*, *RN_Inventory*, *DBH_RN_release*, and *Uncertain_Parameters*. The *Sim_Setup* model component specifies the waste inventory scenario to be simulated. The *Deep_Borehole_Data* model component contains deep borehole-specific data and associated calculations. The *DBH_RN_transport* model component calculates radionuclide transport in the three zones of the deep borehole, and the *DBH_RN_release* model component interfaces between the source-term and borehole transport models. The *Uncertain_Parameters* model component contains all uncertain model parameters. The reference biosphere model [10] is implemented in the *DBH_Results* model component and performs the dose calculations.

Radionuclide transport in the disposal and seal zone is modeled with a series of Goldsim cell pathway elements [11]; each cell element represents a cylinder of the medium of each zone with a length of 20 m and a cross sectional area of 1 m^2. A total of 100 cells are used to simulate radionuclide transport in the disposal zone, and a total of 50 cells for the seal zone. A Goldsim pipe model [11] is used to simulate radionuclide transport in the upper zone having a constant volumetric water flow.

The model is designed to perform a probabilistic analysis, with 100 realizations for each case and for a time period of one million years.

MODEL DEMONSTRATION ANALYSIS

This section analyzes the results of the capability demonstration analysis of the current version of the prototype deep borehole GDS model. The analysis results are presented in terms of the mean radionuclide mass release rate from the major system components (i.e., disposal, seal and upper zones) as the intermediate metrics of performance, and the mean annual dose (mrem/yr) by individual radionuclide at the hypothetical accessible environment. The current model is part of an on-going effort to develop the capability of modeling the deep borehole GDS performance. The use of the mean annual dose is an arbitrary choice to present and discuss the analysis results in order to facilitate a consistent and useful comparison among GDS options. The scientific basis for the results presented is still under development, therefore *should not* be utilized for decision making at this time. The purpose remains a demonstration of modeling capability and as such represents a first look at viability.

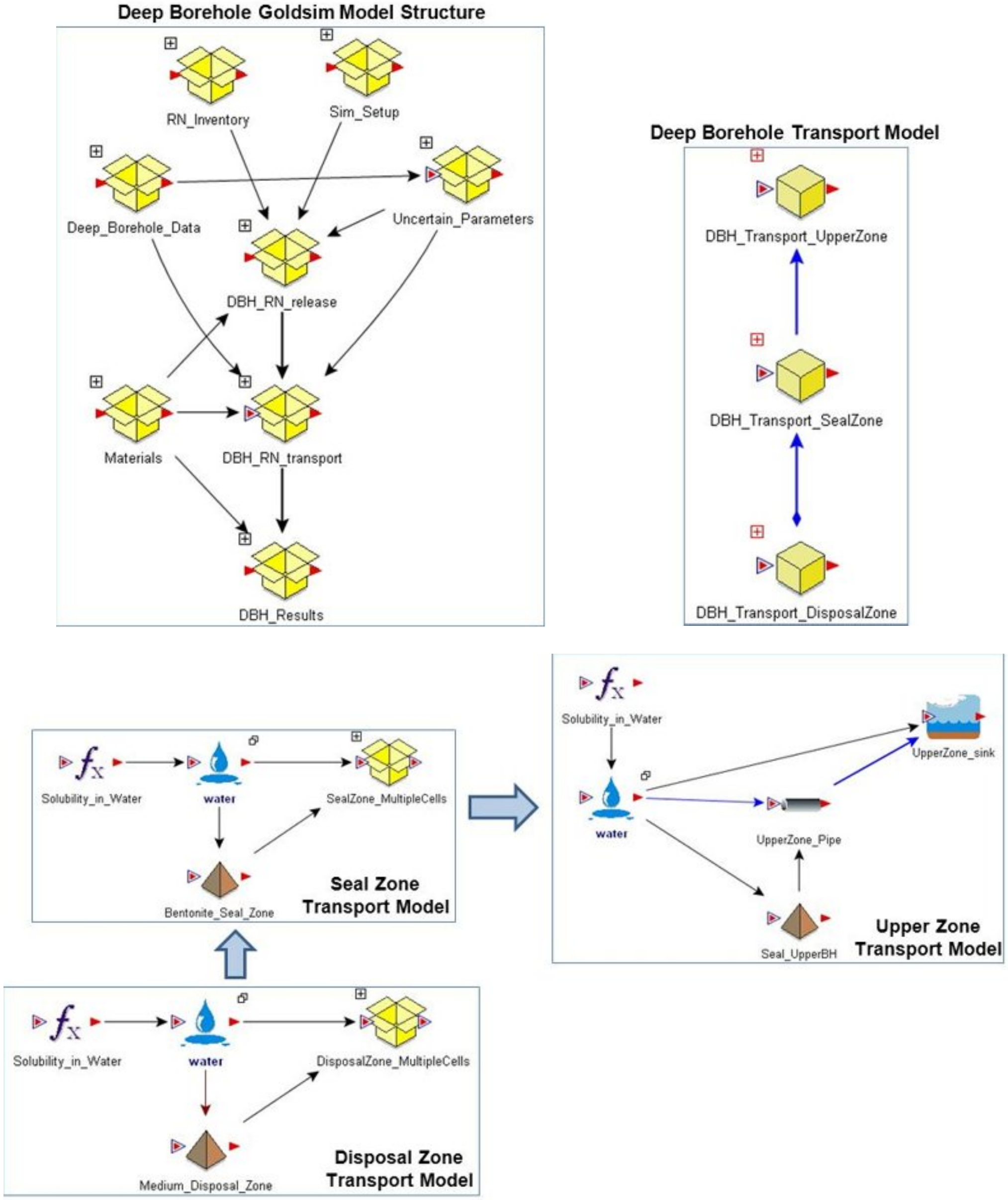

Figure 3. The Goldsim model structure and transport model components of the prototype performance assessment model for a generic deep borehole GDS.

The model demonstration analysis was conducted for two permeability cases: the base permeability case and high permeability case. The base permeability case represents the expected permeability of geologic materials that comprises the deep borehole system and is the reference case. The high permeability case represents a highly conservative bounding condition, for which the system components (e.g., host rock, disturbed rock zone, seals, etc.) have grossly failed, resulting in a much higher permeability than the expected design permeability values. For the base permeability case, the host rock is assigned a permeability of 10^{-19} m^2 (consistent with the properties of crystalline rock at depths greater than 3 km), and the seal and the surrounding annulus of disturbed rock is assigned a value of 10^{-16} m^2. For the high permeability case, a permeability of 10^{-16} m^2 is used for the host rock, and a permeability of 10^{-12} m^2 for the seal and the surrounding disturbed rock. Detailed discussions of the basis for the permeability values and associated modeling approaches are given in Ref. [4].

The analysis was conducted for the waste inventory of 400 disposal canisters of commercial UNF (~150 metric tons of uranium), each containing a single pressurized water reactor (PWR) assembly, vertically stacked down the length of the waste disposal zone (~ 2 km) in a single borehole. The initial radionuclide inventory is representative of PWR fuel assemblies with a burn-up of 60 GWd/MTHM, aged for 30 years [7]. The waste form (commercial UNF) degrades at an annual fractional rate between 10^{-6}/yr and 10^{-8}/yr, consistent with the strongly reducing conditions anticipated in the lower 2,000 m of the borehole [7]. The model demonstration for each case was performed probabilistically, with 100 realizations for a time period of 1,000,000 yr.

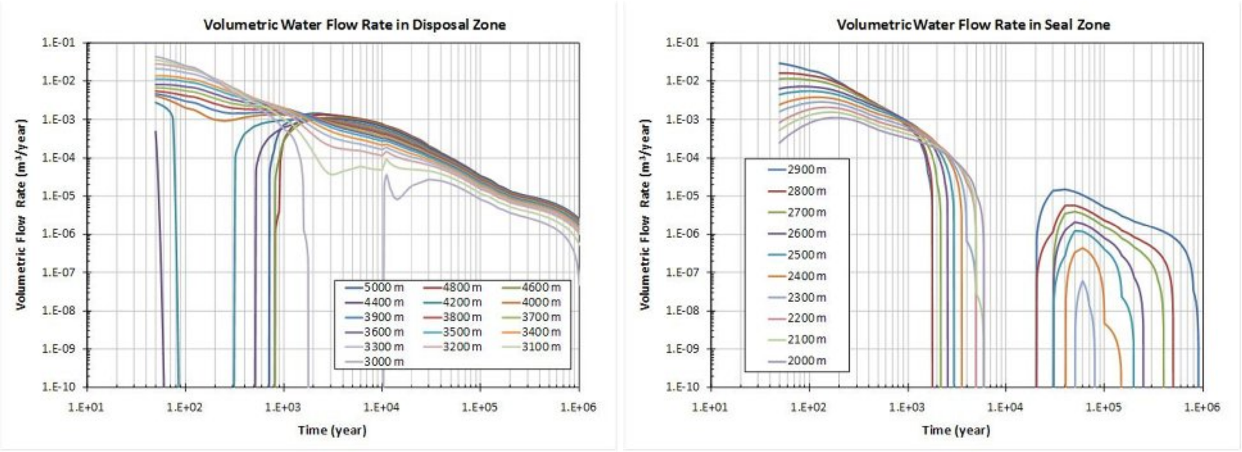

Figure 4. Volumetric water flow rate histories at different locations in the disposal and seal zones for the case of base permeability and commercial UNF waste.

Base Permeability Case Analysis

Figure 4 shows the vertical volumetric water flow rate histories at different locations in the disposal and seal zones for the base permeability case for the disposal of the commercial UNF inventory. The flow rate histories were obtained from detailed thermal hydrologic process-level analysis results and input to the deep borehole GDS model as a look-up table. The volumetric flow rate is for a borehole with the cross-sectional area of 1 m^2. In some instances the flow rates at certain locations and times could be downward directed. For all downward flow rates from the thermal-hydrologic analysis, a very small positive value has been assigned for conservatism and model simplification. The outcome of the adjustment is shown as vertical curves leading to the very small value off the scale of y-axis. For the location and time period corresponding to the arbitrary small value, upward advective water flows are negligibly small, and diffusion is the dominant mechanism to transport dissolved radionuclides in the disposal and seal zones. The simplifications will be removed in the future improvement of the model.

Figure 5 shows results for the mean advective and diffusive radionuclide mass release rates from the disposal zone (i.e., top of the disposal zone). The waste inventory is assumed to be uniformly distributed along the length of disposal zone (i.e., 2,000 m). For most radionuclides the mean advective release rates are higher than the mean diffusive release rates at early times, but the mean diffusive release rates increase with time, exceeding the mean advective release rates in the later time periods. I-129 has the highest mean release rate by both transport mechanisms for the entire analysis time period.

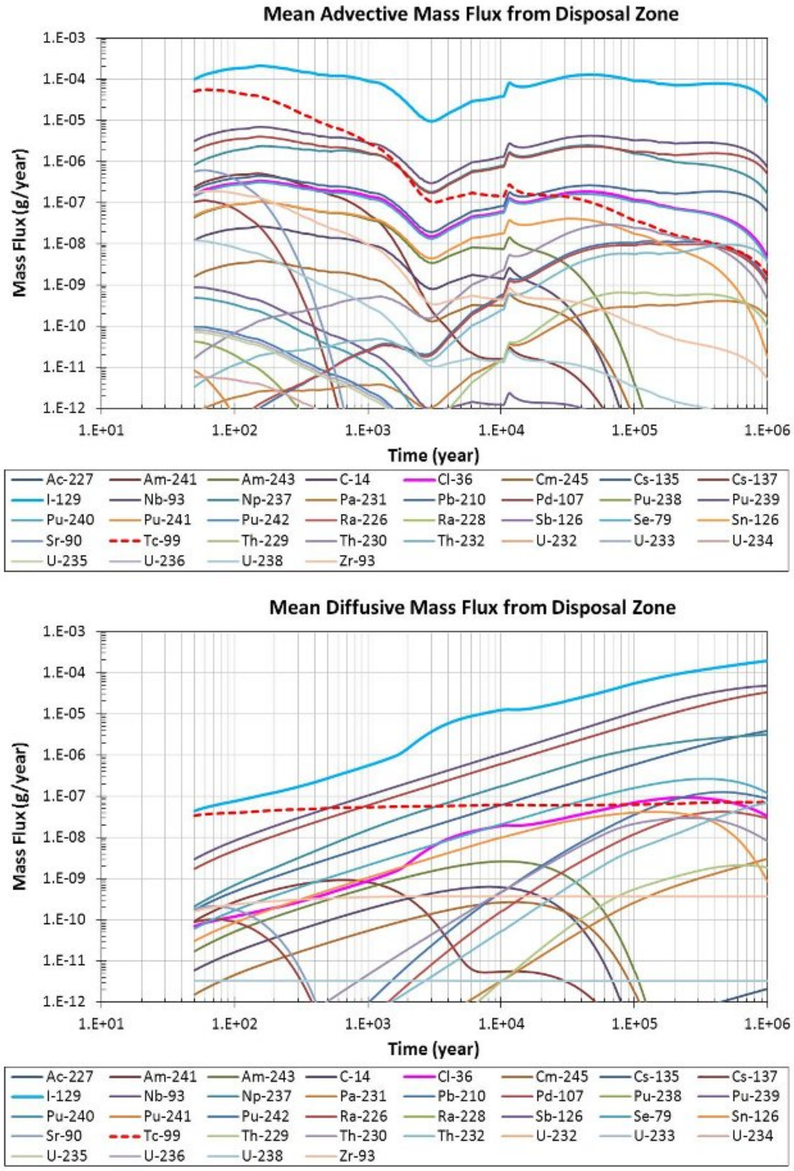

Figure 5. Mean advective and diffusive mass release rate from the disposal zone for the case of base permeability and commercial UNF waste.

Figure 6 shows the mean diffusive mass release rate from the seal zone (i.e., at the top of seal zone). Because of very low upwards water flow rate (especially near the top of seal zone for later time periods) and retardation by sorption, calculated mean advective release rates are negligibly small and not shown in the figure. The mean diffusive release rates are also very low due mainly to sorption on compacted bentonite used in the seal zone. Again, I-129 is the dominant radionuclide in terms of the mean mass release rate.

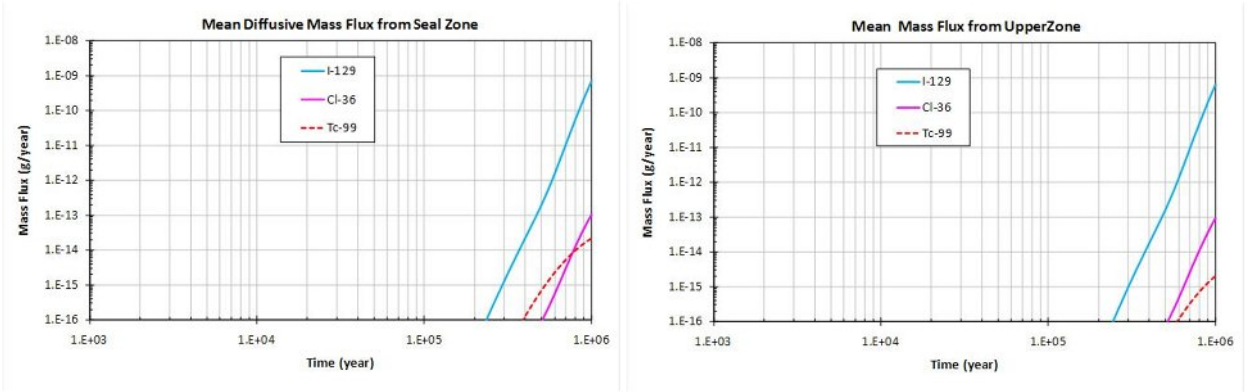

Figure 6. Mean diffusive mass release rate from the seal and upper zone for the case of base permeability and commercial UNF waste.

The impact of radionuclide retardation in the seal zone is shown for the very low mass release rates from the upper zone as shown in Figure 6. As discussed previously, a constant upward volumetric water flow rate of 2.35×10^{-3} m^3/yr is used for the upper zone for the entire analysis time period. The upper zone peak mean release rate for the non-sorbing radionuclides (I-129 and Cl-36) are about the same as the seal zone peak mean release rate; the upper zone mean release rate of Tc-99 is further reduced as it sorbs on the upper zone geologic materials.

Figure 7 shows the mean annual dose by individual radionuclides at the hypothetical accessible environment. I-129 is the dominant annual dose contributor, but the calculated radionuclide mean annual doses are negligibly small.

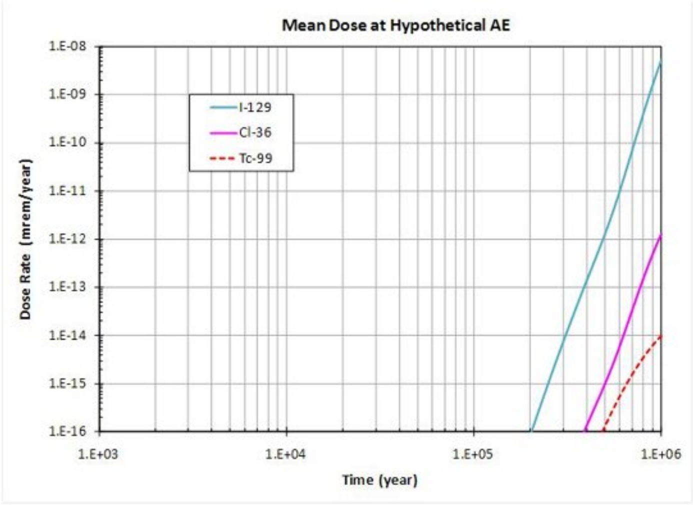

Figure 7. Mean annual dose at the hypothetical accessible environment for the case of base permeability and commercial UNF waste.

High Permeability Case Analysis

As discussed above, sensitivity analyses were conducted to evaluate an assumed condition with a much higher permeability for the system components than the base case permeability. Figure 8 shows the results of the upward volumetric water flow rate histories at different locations in the deep borehole disposal and seal zones for the high permeability case disposing of commercial UNF. As shown in the figure, upward water flows at considerably higher rates than the base permeability case for both zones over the entire simulation time. The same constant upward volumetric water flow rate of 2.35×10^{-3} m^3/yr is also used in the upper zone for the high permeability case. The water flow profiles suggest that advective transport would be the dominant mechanism to move dissolved radionuclides upwards to the surface.

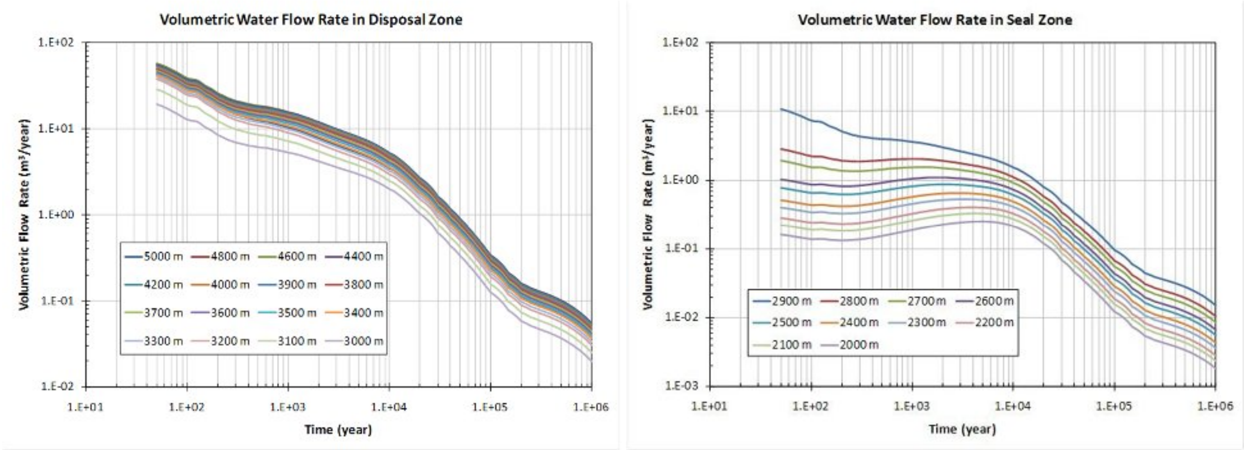

Figure 8. Volumetric water flow rate histories at different locations in the disposal and seal zones for the case of high permeability and commercial UNF waste.

Figure 9 shows the model results for the mean advective and diffusive radionuclide mass release rate from the disposal zone. The waste inventory is uniformly distributed along the length of disposal zone (2,000 m). As expected from the water flow rate profiles, the mean advective release rates are much higher than the mean diffusive release rates for the entire simulation time period. For advective transport in the disposal zone, other radionuclides such as Np-237, Pd-107 and Nb-93 have higher mean release rates than I-129. Note that I-129 is not shown in the diffusive release figure, and this is because I-129 undergoes back-diffusion (i.e., negative diffusion or downward diffusive flux) for the entire analysis time period. The back-diffusion is caused by the large advective flux, which results in higher I-129 concentrations at a higher node than at a lower node. The resulting downward concentration gradient causes the back-diffusion, which is expected process for this condition. The advective component follows the direction of the upward groundwater flux. Np-237 and Cs-135 are two dominant radionuclides in terms of the upwards diffusive release rates.

Figure 10 shows the mean advective and diffusive mass release rate from the seal zone (i.e., at the top of seal zone). I-129 has the highest mean release rate by both diffusion and advection, and the mean advective release rate is much higher than the mean diffusive release rate. The dominance of I-129 is due to the fact that no sorption has been assigned to it and also it has unlimited solubility. Compared to the base permeability case, many other radionuclides (notably Tc-99, Cl-36, Se-79, etc.) are released at considerably high rates.

The mean mass release rates from the upper zone (Figure 11) show that I-129 is the dominant radionuclide and Tc-99 and Cl-36 are also important in terms of the peak mean release rate. A similar trend is shown for the mean annual dose at the hypothetical accessible environment, with I-129 being the dominant annual dose contributor (Figure 12). It is interesting to note that the annual dose contribution by C-14 is high relative to its peak mean mass release rate from the upper zone, and this is the outcome of mainly the high specific activity (4.47 Ci/yr) of the radionuclide.

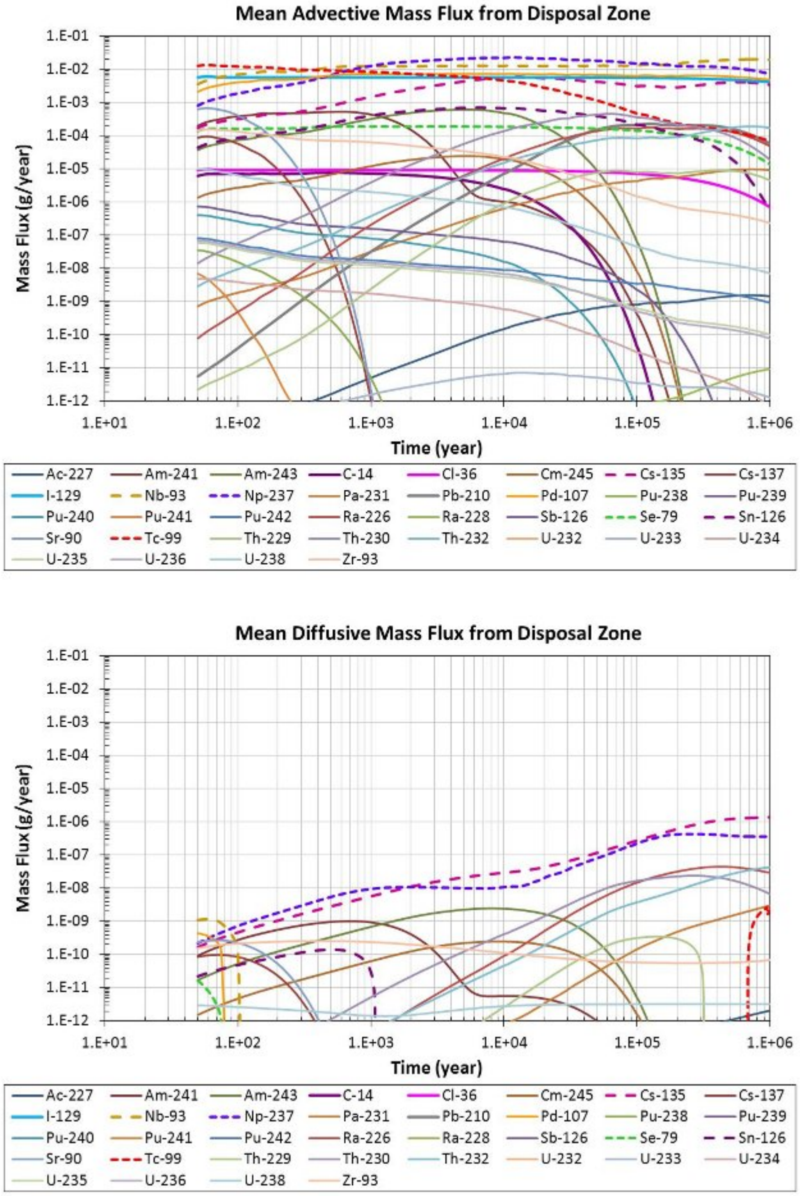

Figure 9. Mean advective and diffusive mass release rate from the disposal zone for the case of high permeability and commercial UNF waste.

The high permeability case is a highly conservative assumption. These preliminary results reinforce the importance of ensuring elimination of potential causes for high upward water flows in a deep borehole, and highlight the importance of a robust seal design in assuring long-term isolation.

SUMMARY AND CONCLUSIONS

A prototype performance assessment model for a deep borehole GDS has been developed using the approach for modeling the performance of a mined geological repository, and the preliminary model results are discussed for the purpose of the model capability demonstration. The current model is the initial outcome of longer term efforts to develop a deep borehole GDS analysis tool and needs further improvement and refinements as the study progresses. The long-term goal of the effort is to develop a highly efficient and flexible analysis tool to evaluate and address, with minimal changes, technical issues associated with the deep borehole GDS options. Although it is preliminary, the current model analysis helps to draw some important considerations for the on-going efforts to develop the deep borehole GDS model and to evaluate the performance.

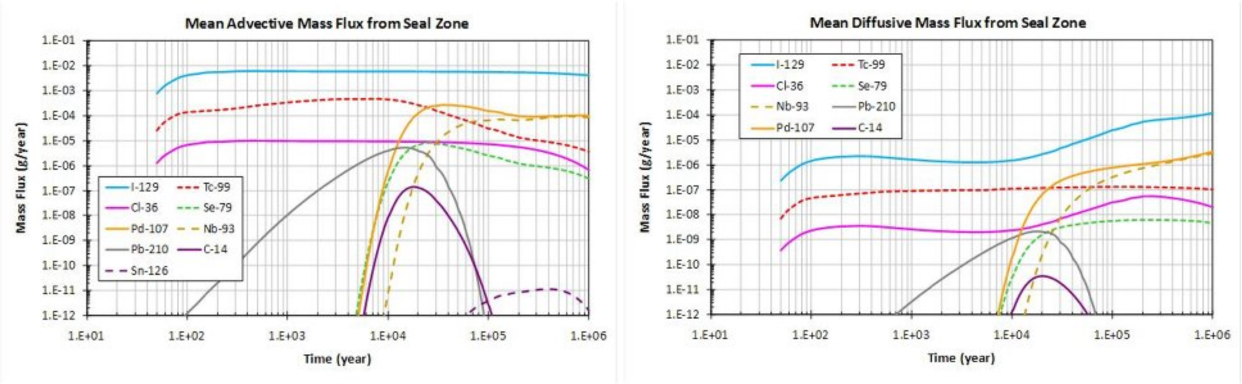

Figure 10. Mean advective and diffusive mass release rate from the seal zone for the case of high permeability and commercial UNF waste.

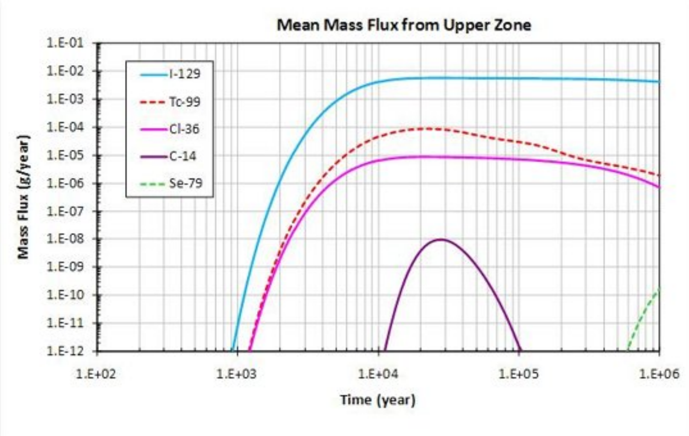

Figure 11. Mean advective mass release rate from the upper zone for the case of high permeability and commercial UNF waste.

The preliminary quantitative results from the simplified deep borehole GDS performance assessment indicate that radionuclide releases from a hypothetical deep borehole repository, and the annual radiation doses to hypothetical future humans associated with those releases, may be extremely small. For the base case values of permeability, radionuclide releases and annual dose rates at the surface are essentially zero. For the high-permeability case with fully degraded seals, the simulated releases and dose rates correspond to an acceptably small risk to human health. While much work needs to be done to validate the model assumptions, these preliminary results highlight the importance of a robust seal design in assuring long-term isolation, and suggest that deep boreholes may be a viable alternative to mined repositories for disposal of both HLW and UNF.

As for a typical mined geological disposal of HLW and UNF, soluble, non-sorbing (or weakly sorbing) fission product radionuclides, such as I-129, Se-79 and Cl-36, are the likely major dose contributors for a deep borehole repository. The current deep borehole GDS performance analysis has also identified the following technical issues and/or knowledge gaps to improve and enhance the confidence of future model analysis.

- Radionuclide release pathways and scenarios are important to the performance analysis of a generic deep borehole repository. Additional studies are needed to improve the conceptual models for the radionuclide release pathways and scenarios that are representative of a deep borehole GDS.
- Geochemical processes in deep borehole environments are challenging and uncertain. Limited data are available for potentially important geochemical processes such as stability and dissolution behavior of radionuclide-bearing mineral phases and sorption of radio-elements to geologic materials under conditions found in deep borehole environments including chemically reducing, high ionic strength brines at elevated temperatures. For example, a majority of the sorption (Kd) values used to model the radionuclide sorption in the current deep borehole GDS model are based on the ambient temperature sorption data. Additional studies and experimental work are needed to better characterize and quantify important geochemical processes in deep borehole environments.
- Additional studies can help characterize and quantify the degradation process of candidate waste forms in generic deep borehole repository environments. The fractional waste form degradation rates used in the current deep borehole GDS model are based on the data for typical mined geologic repository environments. The waste form degradation process and the degradation rate in deep borehole geologic environments could be different from those for mined geologic repository environments. Also, future analysis needs to include the possible rapid release of a gap fraction of mobile radionuclides in the waste form.
- Improved analyses are needed to better define and quantify the waste stream type and inventory, particularly reprocessing HLW of commercial UNF.

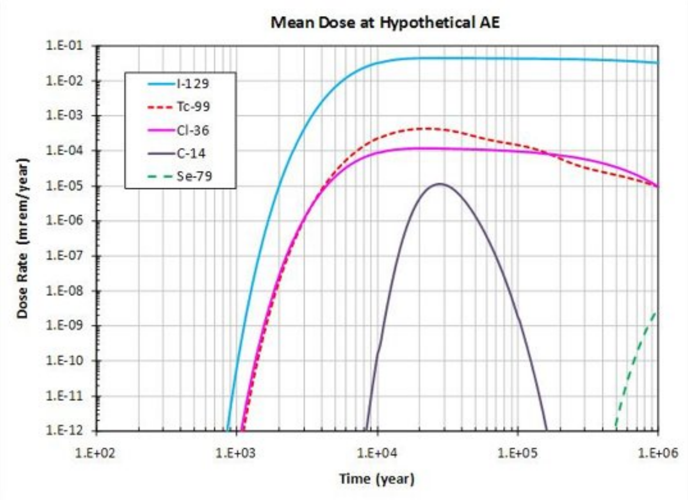

Figure 12. Mean annual dose at the hypothetical accessible environment for the case of high permeability and commercial UNF waste.

REFERENCES

1. Swift, P.N. et al (2011). *Preliminary Performance Assessment for Deep Borehole Disposal of High-Level Radioactive Waste*. Proceedings of the 13th International High-Level Radioactive Waste Management Conference (IHLRWMC), April 10-14, 2011, Albuquerque, NM.
2. Brady, P.V. et al. (2009). *Deep Borehole Disposal of High-Level Radioactive Waste*, Technical Report SAND2009-4401, Sandia National Laboratories, Albuquerque, NM.
3. Arnold, B.W. et al. (2011). *Reference Design and Operations for Deep Borehole Disposal of High –Level Radioactive Waste,* Technical Report SAND2011-6749, Sandia National Laboratories, Albuquerque, NM.
4. Arnold, B.W. et al. (2011). *Thermal-Hydrologic-Chemical-Mechanical Modeling of Deep Borehole Disposal*. Proceedings of the 13th International High-Level Radioactive Waste Management Conference (IHLRWMC), April 10-14, 2011, Albuquerque, NM.
5. Hadgu, Teklu and Bill W. Arnold, 2010, Thermal hydrology modeling of deep borehole disposal of high-level radioactive waste (abstract), American Geophysical Union 2010 Fall Meeting, December 13-17, 2010, American Geophysical Union, Washington, DC.
6. Gibbs, J.S. et al. (2011). *A Multibranch Borehole Approach to HLW Disposal*. Proceedings of the 13th International High-Level Radioactive Waste Management Conference (IHLRWMC), April 10-14, 2011, Albuquerque, NM.
7. Clayton, D., et al (2011). *Generic Disposal System Modeling — Fiscal Year 2011 Progress Report*. Technical Report SAND2011-5828P, Sandia National Laboratories, Albuquerque, NM.
8. Wang, Y., and J.H. Lee (eds.) (2010). *Generic Disposal System Environment Modeling--Fiscal Year 2010 Progress Report*. Prepared for U.S. Department of Energy, Office of Nuclear Energy, Fuel Cycle Research and Development Program. Albuquerque, NM: Sandia National Laboratories.
9. Zyvoloski, G.A., B.A. Robinson, Z.V. Dash, and L.L. Trease (1997). *Summary of the models and methods for the FEHM application, A Finite-Element Heat- and Mass-Transfer Code.* Technical Report LA-13307-MS, Los Alamos National Laboratory, Los Alamos, NM.
10. International Atomic Energy Agency (2003). *Reference Biospheres for Solid Radioactive Waste Disposal.* IAEA-BIOMASS-6, Vienna, Austria.
11. GoldSim Technology Group 2011. *GoldSim version 10.50*.

ACKNOWLEDGEMENT

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. This work is supported by DOE Office of Nuclear Energy Used Fuel Disposition Program. The authors would like to thank Palmer Vaughn at Sandia National Laboratories for his helpful review comments to improve the paper. This paper is Sandia publication SAND2012-0337C.