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MONTE CARLO SIMULATIONS FOR GENERIC GRANITE REPOSITORY STUDIES

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In a collaborative study between Los Alamos National Laboratory (LANL) and Sandia National Laboratories (SNL) for the DOE-NE Office of Fuel Cycle Technologies Used Fuel Disposition (UFD) Campaign project, we have conducted preliminary system-level analyses to support the development of a long-term strategy for geologic disposal of high-level radioactive waste. A general modeling framework consisting of a near- and a far-field submodel for a granite GDSE was developed. A representative far-field transport model for a generic granite repository was merged with an integrated systems (GoldSim) near-field model. Integrated Monte Carlo model runs with the combined near- and far-field transport models were performed, and the parameter sensitivities were evaluated for the combined system. In addition, a sub-set of radionuclides that are potentially important to repository performance were identified and evaluated for a series of model runs. The analyses were conducted with different waste inventory scenarios. Analyses were also conducted for different repository radionuclide release scenarios. While the results to date are for a generic granite repository, the work establishes the method to be used in the future to provide guidance on the development of strategy for long-term disposal of high-level radioactive waste in a granite repository.

I. INTRODUCTION

This paper discusses the development of the granite Generic Disposal System Environment (GDSE) model and presents preliminary model results. For a better comparison among the different disposal environments, a uniform set of assumptions about model configurations is developed and applied to both salt and granite model cases. The reference near field model implemented as a GoldSim template is described in section II.A. The granite GDSE model adopts this template and incorporates an additional module on radionuclide diffusion through the bentonite buffer around waste packages in the near field. The far-field component of the granite GDSE is developed by incorporating the Finite Element Heat and Mass Transfer (FEHM) code [1, 2] into the GoldSim model [3], and is described in section II.B. The system level generic granite GDSE model couples the near field and the far field components for performance assessment simulations. The versions of codes used for this study are: GoldSim (version 10.11) and FEHM (version 3.0).

II. GRANITE GDSE MODEL DESCRIPTION

The model assumes that the repository is located in a saturated, chemically-reducing environment below the water table. For simplification, the repository is assumed to have a square footprint with 25 m spacing between emplacement tunnels and 6 m between waste packages. Three waste types are considered: commercial used nuclear fuel (UNF), existing DOE high level waste (HLW) and reprocessing waste (RW). The model includes 36 radionuclides, accounting for both in-growth of daughters and isotopic mixing among radionuclides. A hypothetical biosphere (the performance measure boundary) is assumed to be located 5 km from the repository edge. The model analysis runs 100 Monte-Carlo realizations for a time period of 1 million years.

Uncertainty in the expected behavior of a generic granite repository requires that the granite GDSE model analyses be probabilistic in order to capture the likely range of potential outcomes. The granite GDSE model evaluates likely future outcomes by conducting multiple realizations using value distributions of uncertain parameters that may be important to a generic granite repository performance. IAEA BIOMASS Example Reference Biosphere 1B (ERB1B) dose model is used to convert the output radionuclide concentrations in the ground water at the hypothetical drinking well location to an estimate of annual dose based on drinking well water consumption [4].

II.A. Near Field of Granite GDSE

The near-field represents physical domains and flow paths that control waste form dissolution and radionuclide transport before radionuclides enter the overlaying aquifer. The near-field model has incorporated the following model components:

- Waste package configurations
- Inventory for different waste types

- Reference repository layout
- Waste form degradation
- Solubility of key radio-elements
- Near-field volume
- Repository waste inventory scenarios
- Repository radionuclide release scenarios

Because the near-field thermal evolution information is not available, the near-field model assumes the site ambient temperature. The current version of the near-field model does not consider performance of waste package.

Waste Package Configurations. The waste cask design for spent nuclear fuels of the German salt disposal program [5] was used for the waste package configurations for the near-field model. The outer diameter of waste package with bentonite buffer (0.36m thickness) is 1.56 m, and the outer length 5.5 m. Each waste package is assumed to hold 10 pressurized water reactor (PWR) commercial UNF assemblies, 5 DOE HLW canisters, or 5 reprocessing HLW canisters. The GDSE analysis does not consider performance of waste package. The waste package configuration is included in the near-field model for use in other model components, including number of waste packages, repository footprint, waste package radionuclide inventory, etc.

Waste Inventory. The waste types included in the analysis are: 1) commercial used nuclear reactor fuels (UNF), 2) existing DOE high-level radioactive waste (HLW), 3) and hypothetical reprocessing HLW of commercial UNF. The near-field model radionuclide inventory analysis was based on the detailed fuel cycle waste inventory analysis. [6]

Commercial UNF Inventory. For the once-through fuel cycle waste inventory analysis, four scenarios were considered to evaluate the projected increases in the commercial light water reactor (LWR) UNF inventory; the scenarios considered were to provide a wide range of LWR fuel inventory for use in future analysis [6]. The near-field model inventory analysis used Scenario 1, which assumes no replacement of existing nuclear generation reactors. Selection of this particular scenario for the near-field model is arbitrary, and it needs to be re-evaluated in future analysis. For this scenario, a total of 140,000 metric tons uranium (MTU) UNF is estimated to be discharged from reactors [6]. Out of the total inventory, 91,000 MTU is for the PWR UNF with an estimated total of 209,000 assemblies. This is equivalent to 0.435 MTU per PWR assembly. For simplification of the near-field model inventory analysis, the total inventory was converted to the equivalent PWR inventory, resulting in a total of 321,540 PWR assemblies. The near-field model assumes that a single waste package contains 10 PWR assemblies, and a total of 32,154 waste packages are needed to dispose of the commercial UNF.

The isotope inventory of the UNF is assumed to be represented by the PWR fuel with a burn-up of 60 GWd/MTIHM, 4.73% enrichment and aged 30 years after discharge from reactor [6]. The resulting isotope inventory for the radionuclides of the commercial UNF included in the near-field model can be found in [7].

DOE HLW Inventory. All existing DOE HLW is assumed to be immobilized in the borosilicate glass logs. The near-field model uses the best-estimate projected total number of DOE HLW canisters reported in the recent fuel cycle inventory analysis; the best estimate projection is 25,016 canisters [6]. The near-field model assumes that each waste package contains 5 HLW canisters, and a total of 5,003 waste packages are needed to dispose of the DOE HLW.

The isotope inventory of the DOE HLW is given in terms of the total radioactivity (C_i) for each radionuclide [6]. The radioactivity was converted to the equivalent mass (m_i) for each radionuclide as follows:

$$m_i(g) = \frac{A_i \cdot t_{\frac{1}{2},i} \cdot MW_i}{0.693 \cdot N_A} \quad (1)$$

Where A_i is the radioactivity of radionuclide i, $t_{1/2,i}$ is the half-life of radionuclide i, MW_i is the molecular weight of radionuclide i, and N_A is the Avogadro constant (6.023×10^{23}). The total mass of radionuclides of the existing DOE HLW is estimated to be 1,759 MT. This results in 0.07 MT of radionuclides per HLW canister, and 0.35 MT of radionuclides per waste package. The resulting isotope inventory per DOE HLW canister and per waste package for the radionuclides included in the near-field model is given elsewhere [7].

Reprocessing HLW Inventory. The recent fuel cycle inventory analysis considered several candidate reprocessing methods for commercial UNF and their potential waste streams [6]. For simplification of the near-field model analysis, the following assumptions were made for "hypothetical" reprocessing of commercial UNF:

- Ninety nine percent (99%) of uranium and plutonium are recovered. All others including transuranic elements and fission products of the commercial UNF inventory (140,000 MTU) remain in the waste streams.
- Reprocessing HLW is immobilized in borosilicate glass as for the DOE HLW.
- Reprocessing HLW is encapsulated at the same radionuclide mass loading as for the DOE HLW (i.e., 0.07 MT radionuclide mass per canister).

Note that the above assumptions result in greater concentrations of fission products in the hypothetical reprocessing HLW than the DOE HLW. The total radionuclide mass of the hypothetical reprocessing HLW is estimated 1,426 MT (after removing 99% of uranium and plutonium). For the radionuclide mass loading of 0.07 MT per canister, this is equivalent to a total of 20,276 canisters. The near-field model assumes that each waste package contains five reprocessing HLW canisters, and a total of 4,055 waste packages are needed for disposal. The resulting isotope inventory per reprocessing HLW canister and per waste package for the radionuclides included in the near-field model is given elsewhere [7].

Reference Repository Layout. For simplification of the near-field model development, it is assumed that repository has a square footprint. Knowing the total number of waste packages (N_{WP}) to be disposed of in the repository, the side length (L_{Rep}) of a square repository footprint can be calculated as follows:

$$\frac{L_{\mathrm{Re}\,p}}{L_{WP}+S_{WP}} \times \frac{L_{\mathrm{Re}\,p}}{S_{drift}} = N_{WP} \tag{2}$$

Where L_{WP} is the length of waste package (5.5 m), S_{WP} is the spacing between waste packages (6 m), and S_{drift} is the spacing between emplacement tunnels (25 m). The waste package configuration is from the package design for the German salt repository program [5]. The waste package spacing and emplacement tunnel spacing were taken from the SKB repository design [8].

Waste Form Degradation. The near-field model includes two types of waste form: commercial UNF matrix and borosilicate glass. The waste form degradation in the near-field analysis is modeled with the annual fractional degradation rates (i.e., fractional degradation rate per year), with a distribution that captures potential range of degradation rates in the GDSE conditions. The granite GDSE near-field is expected to be in water-saturated and chemically reducing conditions with varying degrees of redox conditions of groundwater in contact with the waste form. For the commercial UNF waste form, which is predominantly UO_2, the degradation is modeled with the probabilistic fractional rate model of log-triangular distribution with the mode of $10^{-7}\,yr^{-1}$ and the lower and upper bounds of $10^{-8}\,yr^{-1}$ and $10^{-6}\,yr^{-1}$ respectively. The rate range is from the SKB spent nuclear fuel degradation model for its repository situated in a chemically reducing environment [8]. Potential performance credit of the cladding of commercial UNF as a barrier to radionuclide transport is not considered in the GDSE analysis.

The borosilicate glass waste form degradation is much less sensitive to the redox condition of groundwater contacting the waste form. A probabilistic fractional degradation rate model was developed using the literature data for degradation of similar glasses exposed in geologic environments [9, 10]. The rate model is expressed as log-uniform distribution with the minimum and maximum values of $3.4\times10^{-6}\,yr^{-1}$ and $3.4\times10^{-3}\,yr^{-1}$ respectively.

Near-Field Volume. The amount of groundwater that is available to contact with the waste form and to dissolve released radionuclides is needed to calculate the dissolved concentrations of radionuclides in the near-field. The near-field model conceptualizes the near-field of the granite GDSE as a large uniformly mixed container. This is a reasonable assumption for the scoping analysis, considering that waste package performance is not taken into account and that the entire waste inventory becomes available from the beginning of analysis for interactions with the near-field environment releasing radionuclides into the near-field. In the near-field model, the near-field bulk volume is defined as the square repository footprint area times the height of near-field. The emplacement tunnels of a granite GDSE are likely to maintain the structural shape for an extended period of time after repository closure, and, after degradation of the tunnels, are likely to remain more porous than the host rock. In this respect, the near-field model defines the near-field height twice the waste package outer diameter. The near-field heights so defined in the near-field model are arbitrary and need to be re-evaluated in the future analysis.

The so-defined near-field has two major constituents: 1) degraded engineered materials (e.g., waste form, waste package, backfill, etc.), and 2) host rock. The near-field model calculates the near-field groundwater volume available in each of the two constituents by multiplying the bulk volume of each constituent with its respective porosity. The total groundwater volume available in the near-field is the sum of the water volume in each of the constituents.

Radionuclide Solubility. Radionuclide solubility is an important parameter that controls dissolved concentrations of mobilized radionuclides in groundwater. Radionuclide solubility is affected at varying degrees by various geochemical condition parameters, including redox condition of contacting water, temperature, pH, and presence and concentration of other dissolved species. As an initial effort to address the effect of geochemical conditions on radionuclide solubility, the GDSE analysis considers two redox conditions for groundwater: 1) reducing condition water, and 2) less reducing or slightly oxidizing water. The reducing condition water represents the groundwater in the near-field, and the less reducing or slightly oxidizing water represents the groundwater away from the near-field. The near-field water may experience elevated temperature conditions from the thermal perturbations caused by the decay heat of emplaced waste, but the GDSE analysis assumes the site ambient temperature because the near-field thermal evolution information is not available.

Table 1. Elemental Solubility of Select Radionuclides in Near-Field Water

Element	Distribution Type	Solubility (molal)
U	Triangular	4.89E-08 (min); 1.12E-07 (mode); 2.57E-07 (max)
Pu	Triangular	1.40E-06 (min); 4.62E-06 (mode); 1.53E-05 (max)
Am	Triangular	1.85E-07 (min); 5.85E-07 (mode); 1.85E-06 (max)
Np	Triangular	4.79E-10 (min); 1.51E-09 (mode); 4.79E-09 (max)
Th	Triangular	2.00E-03 (min); 4.00E-03 (mode); 7.97E-03 (max)
Tc	Log-Triangular	4.56E-10 (min); 1.33E-08 (mode); 3.91E-07 (max)
Sn	Triangular	9.87E-09 (min); 2.66E-08 (mode); 7.15E-08 (max)
C, Cl, Cs, I, Se, Sr	n/a	Unlimited solubility

Table 2. Elemental Solubility of Select Radionuclides for Far-Field Water

Element	Distribution Type	Solubility (molal)
U	Triangular	9.16E-05 (min); 2.64E-04 (mode); 7.62E-04 (max)
Pu	Triangular	7.80E-07 (min); 2.58E-06 (mode); 8.55E-06 (max)
Am	Triangular	3.34E-07 (min); 1.06E-06 (mode); 3.34E-06 (max0
Np	Log-triangular	1.11E-06 (min); 1.11E-05 (mode); 1.11E-04 (max)
Th	Triangular	8.84E-06 (min); 1.76E-05 (mode); 3.52E-05 (max)
Sn	Triangular	1.78E-08 (min); 4.80E-08 (mode); 1.29E-07 (max)
C, Cl, Cs, I, Se, Sr, Tc	n/a	Unlimited solubility

Note: Elements Ac, Cm, Nb, Pa, Pd, Ra, Sb, Zr are known to be solubility-limited, but are implemented as unlimited solubility in the near- and far-field model because their solubility calculations have not been completed.

The solubility calculations were performed using two well-studied brines from the WIPP site: 1) a concentrated brines (ERDA-6) derived either from the brine pocket beneath the repository; and 2) a dilute brine (DOE-2_UNC) at the interface between the near field and the far field. The concentrated brine is representative of chemically reducing condition, and the dilute brine of much less reducing condition. The chemical compositions of the two brines are given in [7]. The calculations were performed with computer code EQ3/6 and an enhanced Pitzer thermodynamic database [11]. The elemental solubility of key radionuclides used in the GDSE analysis is given in Tables 1 and 2. Details of the solubility analysis for the representative groundwaters are found elsewhere [7].

Repository Waste Inventory Scenarios. Two waste inventory scenarios were considered in the GDSE analysis: 1) Scenario 1: commercial UNF and DOE HLW; and 2) Scenario 2: DOE HLW and reprocessing HLW. The near-field model has incorporated the two waste inventory scenarios with a simple module to switch from one scenario to another. Scenario 1 considers a total of 37,157 waste packages (32,154 commercial UNF waste packages plus 5,003 DOE HLW waste packages), and a square repository footprint with a side of 3,270 m based on the reference waste package spacing. Scenario 2 considers a total of 9,058 waste packages (5,003 DOE HLW waste packages plus 4,055 reprocessing HLW waste packages) and a smaller square repository footprint (a side of 1,615 m).

Repository Radionuclide Release Scenarios. Two scenarios are considered for radionuclide release from a granite GDSE: the disturbed case and the undisturbed case.

1) The disturbed case represents a non-nominal process that provides a fast pathway for radionuclide release to the far-field from the GDSE, and is modeled by human intrusions. The human intrusion scenario assumes a single borehole penetration through a waste package at 1,000 years after repository closure. The number of waste packages affected (one penetrated plus, if any, neighboring packages affected) is randomly sampled between one and five (uniform distribution). This represents the total amount of waste inventory that becomes available for the fast pathway release by human intrusions.

2) The undisturbed case releases radionuclides by a sequence of nominal processes that are expected to occur in a generic repository. Diffusion through bentonite buffer is considered as one potential undisturbed release scenario. Bentonites have been proposed as buffer material for geological disposal of radioactive waste. In a water-saturated environment, the fluid in the bentonite buffer is almost static because of the very low permeability in the medium, and the advective transport is

negligible. The only significant transport in the near field is the diffusion of radionuclides through the bentonite buffer coupled with radionuclide sorption to bentonite material. Some waste packages may directly intersect with fractures in the surrounding granite rock. Radionuclides released from these waste packages are transported to the aquifer through fast fracture flows.

Separate near-field models were developed and implemented for each of the two release scenarios. For the both scenarios, the near-field model does not consider potential performance benefits of waste packages; that is, waste form starts to degrade at time zero.

II.B. Far Field of Granite GDSE

Reactive transport model – FEHM

The Finite Element Heat and Mass Transfer (FEHM) code [1, 2] is coupled to the GoldSim model to represent the far-field component of the granite GDSE model. This approach enables the full capabilities of FEHM to be employed in the calculation. In many instances, a process model of a component of the natural system will be developed with a full three-dimensional representation using a code like FEHM (e.g. the unsaturated and saturated zone components of the Yucca Mountain system). This capability development, described below, is therefore a significant improvement in our ability to integrate process level models in disposal system analyses.

In this generic, non-site-specific study, no process model is available to integrate into the granite GDSE model. Therefore, a more generic approach to representing the far field is required to capture the key hydrologic, and physical and chemical transport processes. A simple yet flexible far-field pathway model using FEHM has been developed for this purpose. The model consists of radionuclide decay and in-growth, advection, matrix diffusion, and sorption, all features that are implemented using FEHM's reactive transport modeling capability. The advection term is parameterized using a feature that enables the user to prescribe a distribution of advective travel times through a hydrologic pathway. This flexibility enables study of potentially very heterogeneous domains that may give rise to a broad distribution of advective transport times. The user inputs the statistical parameters of the residence time distribution (RTD), or an arbitrary distribution read from a file, and the model automatically constructs a simplified pathway model that reproduces that distribution. We call this approach an RTD-based transport model. The groundwater speed for generic granite GDSE simulations is sampled through stochastic distribution with a mean value of 10 m/yr. On top of the advective component, the model uses FEHM's Generalized Dual Porosity Model (GDPM) feature to include diffusive exchange between the flowing porosity and the surrounding rock matrix. Because the model is established using a numerical modeling approach in FEHM, any other relevant transport process that is included in FEHM is made available as well. In this study, diffusion, radioactive decay and tracking of decay chains, and sorption (with an equilibrium "Kd approach") are used in the results that follow. An extensive theory was developed to implement this RTD-based model, the details of which are provided in FY08 GNEP report Appendix B.1 [12].

FEHM coupled with GoldSim

The FEHM code was modified to couple with GoldSim for probabilistic simulations for granite generic repository studies. In the coupled model, GoldSim performs the overall time steps of the model run, and radionuclide mass is transferred to and from FEHM at each time step. This capability was implemented by using GoldSim Contaminant Transport Module External pathway, which calls FEHM as a dynamic link library (DLL). GoldSim passes a string of variables into each FEHM simulation to initialize the coupled simulation as well as at each GoldSim time step during the system level simulation. These variables include: time, the number of species that FEHM will be simulating, and the amount of mass entering the groundwater pathway.

GoldSim initializes the simulation by passing the first time increment to FEHM. In the FEHM simulation, GoldSim passes into FEHM the mass associated with each radionuclide arriving into the groundwater pathway during that time step. FEHM accepts the incoming mass and adds it to the ongoing calculation of transport through the RTD-based model for the far field pathway to the far-field boundary using the model described above. The cumulative transport of each species, including radioactive decay, is calculated. FEHM can be invoked in a way that enables multiple, smaller time steps to be taken within each GoldSim time steps to ensure that the tracer transport solution converges to an accurate solution. At the end of each GoldSim time step, FEHM passes back into GoldSim any mass reaching the far-field boundary. Mass reaching the far-field boundary is either from the initial input of the primary species from the source region or in-growth of the daughter products formed during transport along the groundwater pathway.

The FEHM input data files contain inputs such as diffusion and sorption parameters that are to be generated from a stochastic distribution. To accomplish this in a flexible way, a DLL was developed to alter the data in the FEHM input files at the beginning of each realization. The DLL INPUTDAT is invoked by GoldSim initially, before GoldSim executes FEHM, to generate an input data file for each FEHM realization run. For each realization, the INPUTDAT program samples the input parameters from a stochastic distribution generated by GoldSim, and places them in the correct places in the input data template to create a new input data file for that

FEHM realization. This development was done in a general way, such that any parameter in the FEHM input file can be generated stochastically and placed into the file at runtime.

III. MODEL RESULTS

This section discusses the preliminary results of the granite GDSE model analysis. The coupling between near field and far field model is handled as follows: far field model takes the total mass flux output from near field model as the input mass flux to carry out the far field transport by FEHM. Parameters for representative radionculides, bentonite buffer, near and far field transport can be found in FY10 Fuel Cycle R&D report [7] Tables 1 through 3. Note that parameter ranges and distributions are selected just for a demonstration purpose of the granite GDSE model analysis, and many of these parameters are site-specific [13-19].

Two independent radionuclides release scenarios are simulated:

1) Disturbed Scenario (human intrusion): Assume a single borehole penetrates through the repository at 1,000 years, thus creating a fast pathway for radionuclide transport to the aquifer. The flow rate up the borehole is sampled through a stochastic distribution with a mean value 2.55 m^3/yr. The number of waste packages affected (i.e., waste inventory affected) by a single borehole penetration is sampled between 1 and 5. Two cases are considered for this scenario:

- Case I: Assume only commercial UNF WPs are affected by human intrusion (HI). No DOE HLW inventory is affected.
- Case II: Assume only DOE HLW WPs are affected by HI. No reprocessing HLW inventory is affected.

2) Undisturbed Scenario (diffusion through bentonite buffer): In this scenario radionuclides released from degrading waste form are transported out of the waste package by diffusion through the bentonite buffer. Some waste packages directly intersect with fractures in the surrounding granite rock, and radionuclides released from these waste packages directly enter into fractures for fast pathway transport. The flow rate upward in the intersected fractures is sampled with a mean value of 0.45×10^{-3} m^3/yr per waste package for commercial UNF and 0.14×10^{-3} m^3/yr per waste package for DOE HLW and reprocessing HLW. For those waste packages releasing radionuclides to the fractures, the model assumes a fraction (between 0.1 and 1 percent) of the affected inventory is available for the advective transport in the fractures, and the fraction is sampled between the bounds. Two cases are considered for this scenario:

- Case I: The inventory considered includes commercial UNF plus DOE HLW
- Case II: The inventory considered includes reprocessing HLW plus DOE HLW

The radionuclide mass fluxes (converted to annual dose) at the location of the hypothetical biosphere (5 km downstream from the repository boundary) were analyzed. The simulations were run for 1 million years with 100 Monte Carlo realizations for each cases listed above.

Breakthrough Curves

Figure 1 shows the mean annual doses by radionuclides at the hypothetical biosphere location (5 km downstream from the repository boundary) for Human Intrusion case, calculated from 100 realizations simulations. The ^{129}I mean annual dose (the highest dose brown color line in Fig. 1) surpasses ^{241}Am, ^{243}Am, ^{239}Pu and ^{240}Pu after a few thousands years, and eventually becomes the dominant contributor toward the end of the 1 million year simulation. The long half-life, high solubility, and weak sorption in the far field of the radionuclide contribute to the high mean dose.

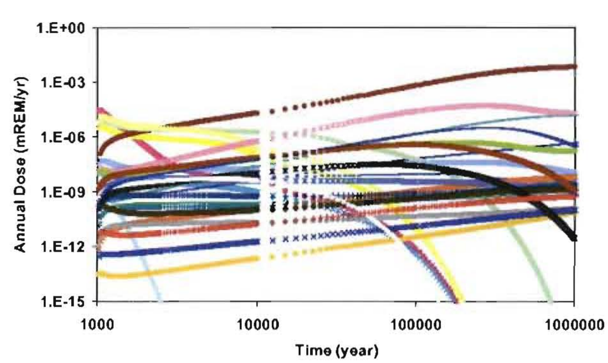


Fig. 1. Mean annual dose (mrem/yr) associated with 100 realizations for 36 individual radionuclide species.

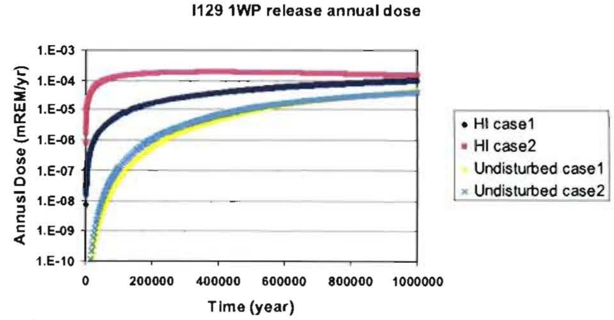


Fig. 2. One waste package release annual dose (mrem/yr) for four simulation cases: human intrusion case I (UNF), human intrusion case II (DOE HLW), undisturbed case I (UNF), and undisturbed case II (DOE HLW).

Figure 2 shows ^{129}I annual mean dose for the cases with one waste package release: human intrusion case I (commercial UNF only), human intrusion case II (DOE

HLW only), undisturbed case I (commercial UNF only) and undisturbed case II (DOE HLW only). Since the DOE HLW glass waste form has a higher degradation rate as compared to the commercial UNF, the human intrusion case II shows the highest mean dose among the four cases. The undisturbed case I and II both show lower mean doses as compared to the human intrusion cases.

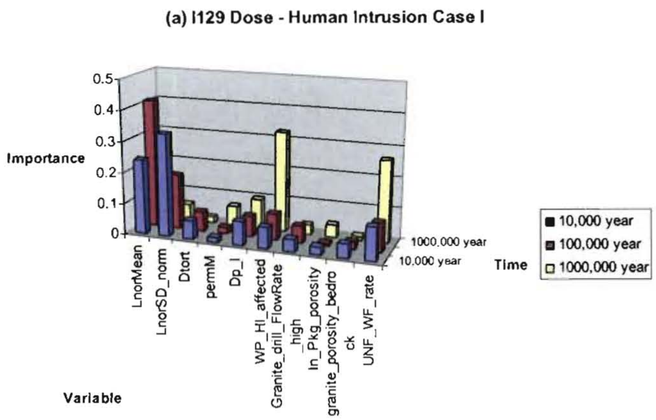
Sensitivity Analysis

A benefit of probabilistic analysis of GDSEs is that the relative importance of various uncertain processes can be examined through a statistical analysis of the Monte Carlo results. This analysis can guide future work planning to reduce uncertainties in the model analysis or in other ways improve the model. Figures 3(a) and 3(b) illustrated this process.

The annual doses were analyzed using a sensitivity analysis tool [20] provided as part of the GoldSim software. The importance analysis of the input variables to the results are statistical measures computed by analyzing multiple realizations of the model in which all of the stochastic variables are simultaneously sampled for each realization of a Monte Carlo simulation. The importance measure is a metric that varies between 0 and 1 representing the fraction of the result's variance that is explained by the variable. This measure is useful in identifying nonlinear, non-monotonic relationships between an input variable and the result (which conventional correlation coefficients may not reveal).

Important parameter uncertainties influencing the overall uncertainty in performance (as measured by the annual dose in this study) depends on the time frame of interest. Each relevant parameter was ranked in order of importance to the overall uncertainty with respect to the annual dose reached at 10^4, 10^5, and 10^6 years. The importance measures shown in following figures are normalized for each time stage so that they can be compared among different time frame of interest.

Figure 3(a) shows that uncertainty in the mean travel time of water in the far field (LnorMean, LnorSD_norm) has dominant influence on uncertainty in the ^{129}I annual dose for most of 1 million year time frame, with decreasing influence toward the end of simulation. The second most important uncertain parameter is the number of affected waste packages (WP_HI_affected) sampled in the near field model, and its influence increases near the end of simulation duration. The third most important uncertain parameter is the commercial UNF waste from degradation rate (UNF_WF_rate), and its influence increases as the simulations proceed towards the end. This shows that at lower UNF fractional degradation rate, for nonsorbing (in far field) radionuclides such as ^{129}I, the annual dose is controlled more by the uncertainties in the near field model than by the uncertainty in the far-field transport.



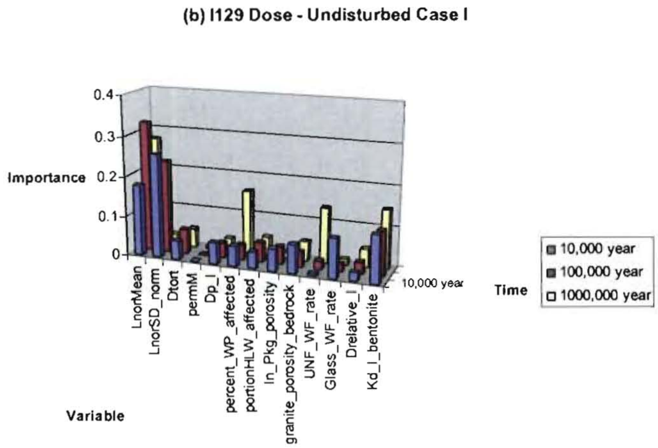


Fig. 3. Importance analysis of input parameters with respect to uncertainties in the ^{129}I annual dose at 5km compliance boundary for (a) Human Intrusion case I (commercial UNF only) and (b) Undisturbed case I (commercial UNF plus DOE HLW). Larger values for a parameter denote that the uncertainties in that parameter have a larger influence on the overall uncertainty in the ^{129}I annual dose.

Figure 3(b) shows the similar situation for ^{129}I annual dose with mean travel time in far field as the top uncertainty parameter. In this case, DOE HLW glass degradation rate (Glass_WF_rate) shows strong influence at the earlier stage of simulation while the commercial UNF degradation rate (UNF_WF_rate) shows strong influence toward the end of simulation. Also the ^{129}I sorption coefficient for bentonite buffer (Kd_I_bentonite) shows a comparable effect as the number of waste packages affected and the waste form degradation rates with respect to uncertainty in the annual dose, and with a relative strong influence through out the entire simulation duration.

IV. CONCLUSIONS

The GDSE model and the results presented in this paper are preliminary and therefore not indicative of the performance of an actual geologic disposal environment or the potential radiation exposures that could occur in that environment. Rather, they can be used to identify the important processes that may affect repository performance. The intermediate applications of this model may include:

- Identifying which radionuclides are important to the disposal system performance;
- Determining which processes (i.e., solubility, linear sorption) significantly affect the disposal system performance;
- Determining how a waste form with a specific radionuclide inventory affects the disposal system performance;
- Determining how the waste form durability affects the disposal system performance.

Future work includes continual improvement of the existing model by incorporating more detailed processes and performing comparative studies among the different disposal environments.

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