Status Report on Reference Case for Generic Disposal System Modeling in Granite

Fuel Cycle Research & Development

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☐ Technical Review	☐ Peer Review
Technical Review (TR)	**Peer Review (PR)**
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☐ Signed TR Report or,	☐ Signed PR Report or,
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STATUS REPORT ON REFERENCE CASE FOR GENERIC DISPOSAL SYSTEM MODELING IN GRANITE

1. Introduction

This report discusses the reference case and performance assessment study conducted for the Generic Disposal System Environment (GDSE) model for granite described in UFD FY11 report [1]. The computer codes used for this study are: GoldSim (version 10.5) [2] and The Finite Element Heat and Mass Transfer (FEHM) code (version 3.0) [3, 4]. The report includes two main sections: 1) reference case design and flow simulation for the generic granite disposal system modeling; 2) generic granite system model performance assessment (PA) study using reference case flow simulation results for far field transport calculation. Monte Carlo simulations with the combined near- and far-field transport models are performed. The dose rates for a subset of radionuclides that could be potentially important to repository performance are calculated. The analyses are conducted for undisturbed radionuclide release scenario.

2. Generic Granite Disposal System Model Description

The generic granite disposal system model is composed of two major subsystems, the near field and the far field.

The near field subsystem encompasses waste form and the EBS (Engineered Barrier System) and the interface with, and the adjacent portion of, the host rock; it includes:

- Repository layout and waste package (WP) configurations
- Radionuclide inventory and waste form degradation
- Solubility control and radionuclide release from waste panels
- Solubility control at the near-field and far-field interface

Current version of the model considered two radionuclide release scenarios:

- Disturbed - Human intrusion
- Undisturbed - Diffusion through bentonite buffer

The far-field component represents contaminant transport through the natural system from the near field host rock to hundreds or thousands of meters; it includes key physical, chemical and hydrological processes such as:

- Radionuclide decay and ingrowth
- Advection (RTD residence time distribution-based transport model to enable the study of potentially very heterogeneous domains)
- Matrix diffusion (GDPM generalized dual porosity model, diffusive exchange between flowing porosity and surrounding rock matrix)
- Sorption

The model assumes that the repository is located in a chemically-reducing environment below the water table. The repository is assumed to have a square footprint with 25 m spacing between emplacement tunnels and 6 m between waste packages. The options for the waste stream being considered are used nuclear fuel (UNF) and high-level radioactive waste (HLW). Types of HLW include DOE high-level radioactive waste (DHLW) and commercial high-level radioactive waste (CHLW) generated from hypothetical reprocessing of commercial UNF. The waste type used for this study is UNF. The near-field model radionuclide inventory analysis is based on the detailed fuel cycle waste inventory analysis conducted for the UFD project [5]. The current version of the near-field model does not consider performance of waste package and Excavation Damage Zone (EDZ).

The FEHM code is coupled into the GoldSim system level model to represent the far field component [6]. The far-field component of the granite GDSE 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.

Two scenarios are considered for radionuclide release from granite GDSE: the disturbed case and the undisturbed case. 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 with a stylized human intrusion. 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. For this study, the undisturbed scenario is considered.

A hypothetical biosphere (the performance measure boundary) is assumed to be located at a certain distance from the repository edge. 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 [7].

The system level generic granite GDSE model couples the near field and the far field components for performance assessment simulations. The granite GDSE model evaluates likely future outcomes by conducting Monte Carlo multi-realization probabilistic simulations with Latin Hypercube sampling. Sensitivity analyses can be performed for probability distributions of uncertain parameters that may be important to a generic granite repository performance. The key model parameters are listed in Table 1. Other parameters and more detailed description of the granite GDSE model can be found in UFD FY11 report [1].

Table 1. Key model parameters

Parameter[1]	**Stochastic Parameter type**	**Base Case Value**	**Distribution Parameters**
UNF matrix degradation rate (1/yr)	Log-triangular	1.528×10^{-7}	1×10^{-8}, 1×10^{-7}, 1×10^{-6}
DHLW degradation rate (borosilicate glass) (1/yr)	Log-uniform	4.917×10^{-4}	3.4×10^{-6}, 3.4×10^{-3}
Porosity, inside waste package	Constant	0.175	N/A
Porosity, bed rock	Uniform	0.00525	Range: 0.0005-0.01
Waste package temperature (ºC)	Constant	25	N/A
Waste package size outer diameter (m)	Constant	0.863	N/A
Waste package size outer length (m)	Constant	5.096	N/A
Inventory Number of waste packages-UNF	Constant	140,000 MTU 32,154 WPs	N/A
Inventory Number of waste packages-DHLW	Constant	1,759 MT 5,003 WPs	N/A
Percent of total waste packages affected by canister failure and diffuse through bentonite buffer	Uniform	0.55%	Range: 0.1% - 1%
Water flow rate to fracture intersecting waste package in undisturbed scenario (m^3/yr/per WP)	Normal	5.1×10^{-4}	mean=$5.1e^{-4}$, stdv=$0.2e^{-4}$
Bentonite buffer thickness (m)	Constant	0.36	N/A
Bentonite density (kg/m^3)	Triangular	1562	1484, 1562, 1640
Bentonite porosity	Triangular	0.435	0.41, 0.435, 0.46
Fracture aperture (m)	Uniform	$2.55e^{-4}$	Range: $1e^{-4}$ - $5e^{-4}$
Fracture spacing (m)	Constant	25	N/A
Solubility (mg/L) for C, Cl, Cs, I, Sr and Pb		unlimited	

[1] Parameters source: (Clayton et al. 2011 [1], Mariner et al. 2011 [8], SKB 2010 [9])

3. Reference Case Design and Flow Simulation

The schematic diagram of the generic granite reference case domain is shown in Figure 1. The domain is chosen as a thin three dimension volume with X direction of 1000 meters, Y direction of 1 meter and Z direction of 600 meters for studying the flow pattern in vertical cross-section. Reference temperature is assumed to be 15 degree C, reference air pressure is assumed to be 0.1 MPa. The reference case simulates a generic granite repository sited in a granite environment. The black small block in Figure 1 at about 300 meter depth level on the left side of the domain represents the repository. The tilted black bar at right side represents a fractured deformation zone.

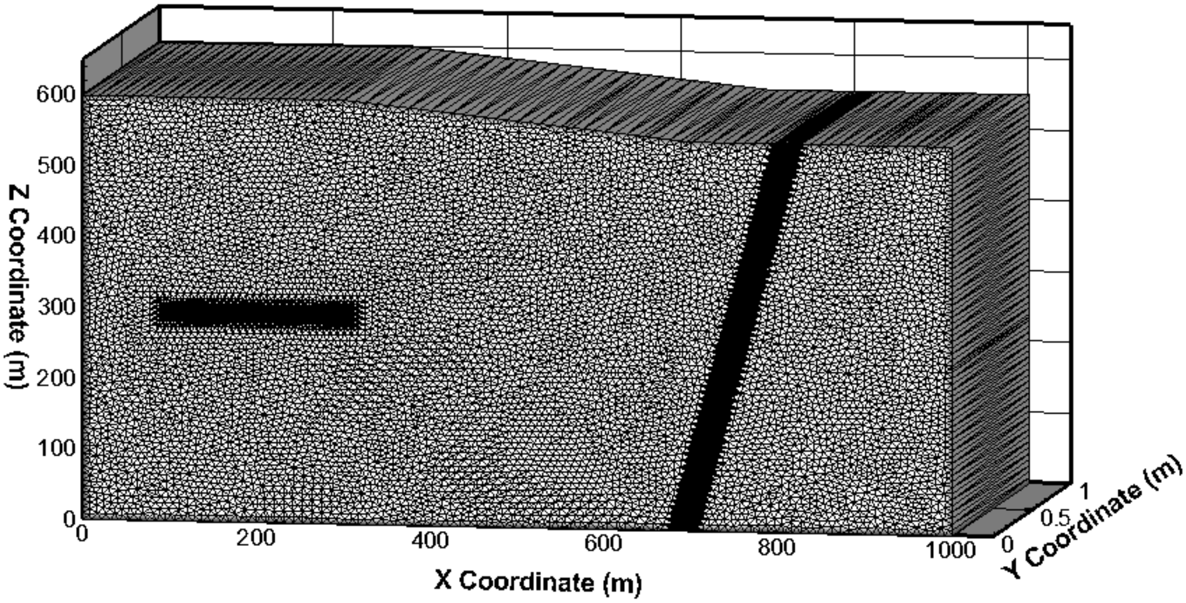

Figure 1. Schematic diagram for the generic granite reference case domain.

Figure 2 shows the design of the reference case and flow simulation with different material zones for the site. The parameters for each zone are listed in Table 2.

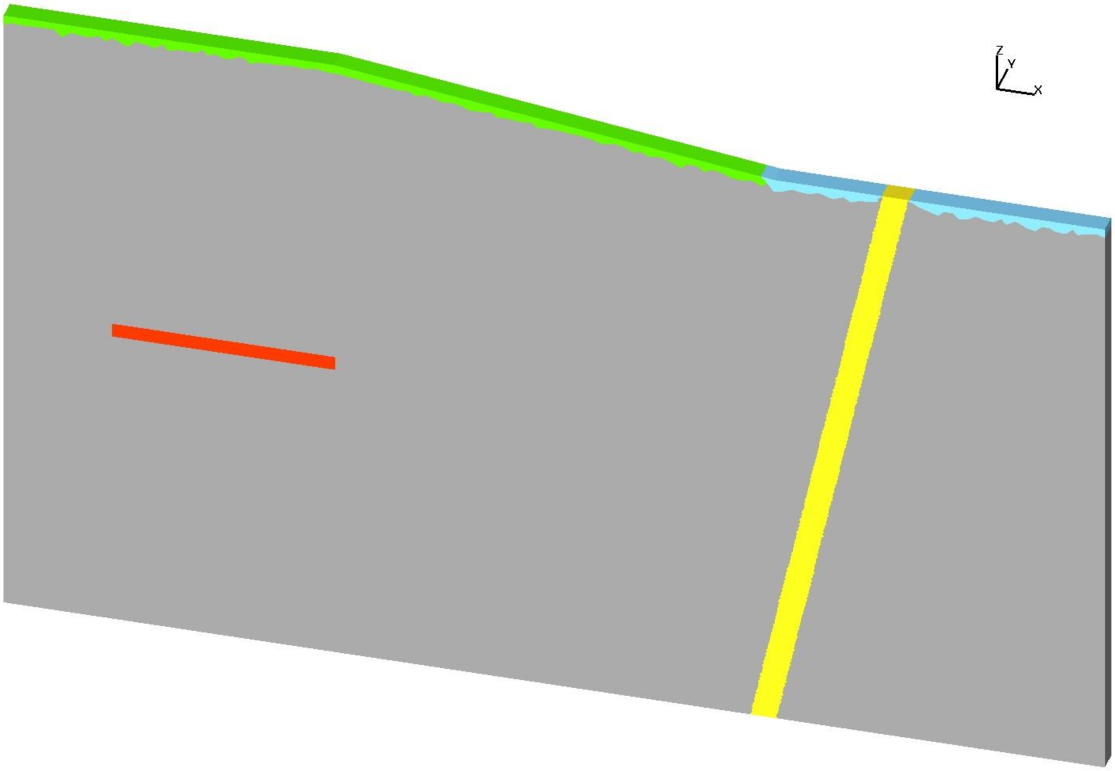

Figure 2. Material zones plot for the reference case domain.

Zone 1 - The top infiltration zone (green color zone: x = 0 to 700m; y = 0m to 1m; z = 600m flat for x = 0m to 300m, then slope down to 550m for x=300m to 700m). Infiltration (100 mm/yr) is introduced into the domain from this higher elevation region.

Zone 2 - The outflow zone (turquoise color zone including top of yellow color zone: x = 700m to 1000m; y = 0m to 1m; z = 550m flat for x=700m to 1000m). The water is allowed discharged only from this lower elevation region (for example, a shallow lake). All other domain boundaries are assumed to be no-flow boundaries.

Zone 3 - The repository zone (red color zone: x = 100m to 300m; y = 0m to 1m; z = 295m to 305m). Radionuclides are assumed released from this region.

Zone 4 - Deformation zone (yellow color zone: tilted area of 20m width with x = 700m to 1000m at the bottom of domain, and x = 800m to 1000m at the top of domain; y = 0m to 1m; z = 0m to 550m). This is an intensely fractured region where most radionuclides will go through.

Zone 5 - Rest of domain bedrock zone (grey color zone for the rest of domain: note the repository zone and deformation zone have finer grid in the model comparing to the rest of bedrock zone).

Table 2. Parameters for the generic granite reference case flow simulation

Parameter	Repository zone	Deformation zone	Bedrock zone
Permeability (m^2)	10^{-14}	10^{-12}	10^{-13}
Density (kg/m^3)	2380	2380	2700
Porosity	0.005	0.05	0.01

With the reference case design, the model simulates how the flow is driven by variations in domain topography (as shown by the steady state flow velocity vectors in Figure 3) as the infiltration getting into the higher terrain (left side top of the domain). Water flow down through repository region (assumed lower permeability than surrounding bed rock) and an intensely fractured deformation region (assumed higher permeability in comparison to the surrounding bedrock), and eventually reach the lower elevation shallow lake at the right side surface of the domain.

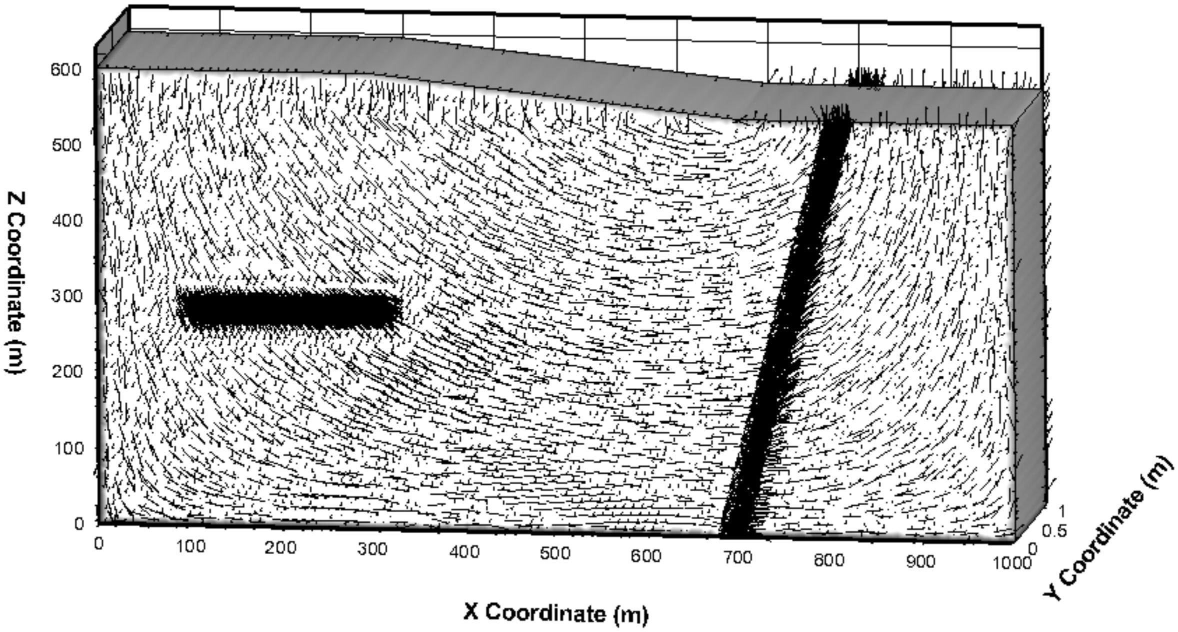

Figure 3. Generic granite reference case steady state flow pattern.

4. Generic Granite System Model Performance Assessment Results

This section discusses using reference case flow simulation results from section 3 for far field transport calculation to carry out generic granite system model performance assessment (PA) study.

Contaminant transport assessment requiring predictions of arrivals at a location downstream is conveniently formulated in terms of the travel time or residence time distribution (RTD). The RTD is a compact way to describe the composite behavior of fluid moving through a groundwater flow system, even when the underlying processes of heterogeneous flow, fast pathways, and hydrodynamic dispersion are complex and uncertain. By adopting an RTD-based approach, the essential features of the flow system can be represented, and in the case of linear solute transport processes, the information is sufficient to obtain a unique prediction of solute breakthrough [10]. Even for nonlinear reaction processes, the RTD is still a fundamental determinant of transport behavior, because it captures the degree of spreading in time of a mass input. Therefore, modeling methods based on the RTD provide an attractive approach for representing results from large-scale, complex process models of the groundwater pathway. For generic studies for which detailed models are not available, an RTD-based approach is also appropriate because it provides a more flexible way to represent flow complexities than a simplified one-dimensional advection-dispersion equation. Detailed discussion about Residence Time Distribution (RTD) Mixing Model (RTDMM) method can be found in Ref. [11].

Assuming radionuclides released from repository (zone 3 in Figure 2) through undisturbed scenario, a hypothetical biosphere (the performance measure boundary) is assumed to be located at ground surface (zone 2 in Figure 2). The RTD function for the far field transport from the releasing site to the biosphere is calculated from the reference case flow simulation results using particle tracking capability in FEHM [3, 4]. The RTD changes with both radionuclides release location and infiltration rate, for this study, it is assumed that the release location to be at middle of repository zone along the repository footprint (x = 100m to 300m, y = 0 to 1m, z = 300m), infiltration to be 100 mm/yr as a conservative assumption. Using the RTDMM method described above, advective travel times are input directly into the generic granite system model in the form of an RTD, allowing other transport processes such as diffusion into stagnant zones and sorption to be readily included.

Using reference case flow simulation derived RTD as the far field transport input, the deterministic performance assessment simulations with each uncertain parameter represented by its mean value are carried out for the generic granite system model. Table 3 lists far field transport parameters for a subset of radionuclides that could be potentially important to repository performance. Parameters for representative radionuclides are summarized in Table 4.

Table 3. Far field transport parameters for radionuclide species

Transport Parameter	Stochastic Parameter type	Base Case Value	Distribution Parameters
Diffusive Tortuosity τ_D, all species	Normal distribution for $\tau_D = D / D_{free}$	$1.172\text{x}10^{-2}$	$1.172\text{x}10^{-2}$, $1.0\text{x}10^{-2}$
Free-Water diffusion coefficient D_{free} (m^2/s), Am	Constant	$9.49\text{x}10^{-10}$	N/A
D_{free} (m^2/s), C	Constant	$1.18\text{x}10^{-9}$	N/A
D_{free} (m^2/s), Pa	Constant	$6.04\text{x}10^{-10}$	N/A
D_{free} (m^2/s), Ra	Constant	$8.89\text{x}10^{-10}$	N/A
D_{free} (m^2/s), Th	Constant	$5.97\text{x}10^{-10}$	N/A
D_{free} (m^2/s), Sn	Constant	$1.55\text{x}10^{-9}$	N/A
D_{free} (m^2/s), Cl	Constant	$2.03\text{x}10^{-9}$	N/A
D_{free} (m^2/s), Cs	Constant	$2.06\text{x}10^{-9}$	N/A
D_{free} (m^2/s), I	Constant	$2.05\text{x}10^{-9}$	N/A
D_{free} (m^2/s), Np	Constant	$6.18\text{x}10^{-10}$	N/A
D_{free} (m^2/s), Se	Constant	$1.04\text{x}10^{-9}$	N/A
D_{free} (m^2/s), Sr	Constant	$7.91\text{x}10^{-10}$	N/A
D_{free} (m^2/s), Tc	Constant	$1.95\text{x}10^{-9}$	N/A
D_{free} (m^2/s), U	Constant	$6.64\text{x}10^{-10}$	N/A
Matrix diffusion coefficient (pore diffusivity) D (m^2/s), Cl	Truncated normal distribution	$1.37\text{x}10^{-10}$	Range:$3.75\text{x}10^{-11}$-$3.21\text{x}10^{-10}$, $1.37\text{x}10^{-10}$, $1.08\text{x}10^{-10}$
D (m^2/s), Cs	Truncated normal distribution	$2.11\text{x}10^{-10}$	Range:$1.03\text{x}10^{-10}$-$3.75\text{x}10^{-10}$, $2.11\text{x}10^{-10}$, $1.05\text{x}10^{-10}$
D (m^2/s), I	Truncated normal distribution	$1.57\text{x}10^{-10}$	Range:$7.96\text{x}10^{-11}$-$3.38\text{x}10^{-10}$,

			$1.57x10^{-10}$, $6.02x10^{-10}$
D (m^2/s), Np	Truncated normal distribution	$6.99x10^{-11}$	Range:$2.8x10^{-11}$-$1.1x10^{-10}$, $6.99x10^{-11}$, $2.75x10^{-11}$
D (m^2/s), Pu	Truncated normal distribution	$4.1x10^{-11}$	Range:$2.61x10^{-11}$-$5.63x10^{-11}$, $4.1x10^{-11}$, $1.07x10^{-11}$
D (m^2/s), Se	Truncated normal distribution	$8.93x10^{-11}$	Range:$8.26x10^{-11}$-$9.46x10^{-11}$, $8.93x10^{-11}$, $5.0x10^{-12}$
D (m^2/s), Sr	Truncated normal distribution	$6.65x10^{-11}$	Range:$2.86x10^{-11}$-$4.0x10^{-10}$, $6.65x10^{-11}$, $9.66x10^{-11}$
D (m^2/s), Tc	constant	$4.2x10^{-12}$	N/A
D (m^2/s), U	Truncated normal distribution	$5.14x10^{-12}$	Range:$3.14x10^{-12}$-$6.29x10^{-12}$, $5.14x10^{-12}$, $1.42x10^{-12}$
D (m^2/s), Ac	Constant	$5.0x10^{-11}$	N/A
D (m^2/s), Pb	Constant	$5.0x10^{-11}$	N/A
D (m^2/s), Sb	Constant	$5.0x10^{-11}$	N/A
D (m^2/s), Zr	Constant	$5.0x10^{-11}$	N/A
D (m^2/s), Nb	Constant	$5.0x10^{-11}$	N/A
D (m^2/s), Pd	Constant	$5.0x10^{-11}$	N/A
D (m^2/s), Cm	Constant	$5.0x10^{-11}$	N/A
Matrix sorption coefficient K_d (cc/g), Ac	CDF	3000	(1000,0) (3000,0.5) (5000,1)
K_d (cc/g), Am	CDF	3000	(1000,0) (3000,0.5) (5000,1)
K_d (cc/g), C	CDF	1	(0.5,0) (1,0.5) (2,1)
K_d (cc/g), Cl	Non-sorbing	0	N/A
K_d (cc/g), Cm	CDF	3000	(1000,0) (3000,0.5) (5000,1)
K_d (cc/g), Cs	CDF	50	(10,0) (50,0.5) (100,1)

K_d (cc/g), I	Non-sorbing	0	N/A
K_d (cc/g), Nb	CDF	1000	(500,0) (1000,0.5) (3000,1)
K_d (cc/g), Np	CDF	5000	(1000,0) (5000,0.5)(10000,1)
K_d (cc/g), Pa	CDF	1000	(500,0) (1000,0.5) (5000,1)
K_d (cc/g), Pd	CDF	10	(1,0) (10,0.5) (50,1)
K_d (cc/g), Pu	CDF	5000	(1000,0) (5000,0.5)(10000,1)
K_d (cc/g), Ra	CDF	20	(10,0) (20,0.5) (100,1)
K_d (cc/g), Se	CDF	1	(0.5,0) (1,0.5) (5,1)
K_d (cc/g), Sn	CDF	1	(0,0) (1,0.5) (10,1)
K_d (cc/g), Sr	CDF	0.2	(0.1,0) (0.2,0.5) (1,1)
K_d (cc/g), Tc	CDF	1000	(300,0) (1000, 0.5) (3000,1)
K_d (cc/g), Th	CDF	5000	(1000,0) (5000,0.5)(10000,1)
K_d (cc/g), U	CDF	5000	(1000,0) (5000,0.5)(10000,1)
K_d (cc/g), Zr	CDF	1000	(500,0) (1000,0.5) (3000,1)
K_d (cc/g), Pb	Constant	0	N/A
K_d (cc/g), Sb	Constant	0	N/A

Parameters source: (Carbol and Engkvist, 1997 [12]; JAEA database [13]; Chu et. al. 2008 [6]). For Ac, Pb, Sb, Zr, Nb, Pd and Cm, diffusion parameters were not readily available (sorption parameters are not readily available for Pb, Sb), and because the model analysis was performed for a generic repository to investigate the feasibility of the modeling system, placeholder values for diffusion and a sorption coefficient of 0 were used for expediency.

Table 4. Parameters for representative radionuclides

Species ID	**Atomic Weight (g/mol)**	**Half-life (year)**	**Solubility (mol/L)**	**Far field sorption coefficient Kd (cc/g)**	**Specific activity (Ci/g)**	**Dose conversion factor (Sv y^{-1} / Bq y^{-1})**
Actinide Parent Species						
Np	237	2.14×10^{6}	1.0×10^{-9}	5000	0.00070487	1.33×10^{-11}
Pu	238	87.7	2.0×10^{-7}	5000	17.127	2.76×10^{-11}
	239	2.41×10^{4}			0.062066	3.00×10^{-11}
	240	6.54×10^{3}			0.22776	3.00×10^{-11}
	242	3.76×10^{5}			0.0039289	2.88×10^{-11}
Am	241	432	6.0×10^{-6}	3000	3.4338	2.40×10^{-11}
	243	7.37×10^{3}			0.19962	2.41×10^{-11}
U	232	68.9	4.0×10^{-10}	5000	22.365	6.7×10^{-11}
	233	1.59×10^{5}			0.0096498	6.12×10^{-12}
	234	2.45×10^{5}			0.0062357	5.88×10^{-12}
	235	7.04×10^{8}			2.1609×10^{-6}	5.68×10^{-12}
	236	2.34×10^{7}			6.4736×10^{-5}	5.64×10^{-12}
	238	4.46×10^{9}			3.3679×10^{-7}	5.81×10^{-12}
Fission Products and Others						
Tc	99	2.13×10^{5}	3.0×10^{-8}	1000	0.016953	7.68×10^{-14}
I	129	1.57×10^{7}	unlimited	0	0.00017651	1.32×10^{-11}
Cs	135	2.3×10^{6}	unlimited	50	0.0011514	2.40×10^{-13}
Se	79	3.27×10^{5}	4.0×10^{-8}	1	0.013839	3.48×10^{-13}
Cl	36	3.01×10^{5}	unlimited	0	0.032991	1.116×10^{-13}

Parameters source: (Clayton et al. 2011 [1], Mariner et al. 2011[8])

In the undisturbed scenario, radionuclides released from degrading waste form are transported away from the waste package by diffusion through the bentonite buffer; the advective transport through it is negligible [9]. Some waste packages directly intersect with fractures in the surrounding granite rock, and radionuclides released from these waste packages enter into the fractures for fast pathway transport. For those waste packages releasing radionuclides to the fractures, the model assumes that a fraction (0.1% to 1%) of the considered inventory is available for the advective transport in the fractures, and the fraction is sampled uniformly between the bounds. The small fraction of waste packages with potential release paths is consistent with detailed analyses from the SKB program [9].

The waste type included in this simulation is used nuclear fuel (UNF). The model calculates the radionuclide mass fluxes out of one waste package by following the transport through the near field and far field, and then sums the doses for affected UNF packages at the end of transport pathway. Far field transport is using RTD calculated from reference case flow simulation discussed in section 3. The model uses granite solubility from Table 2-5 of Ref. [8] for granite at 25°C.

The radionuclide mass fluxes (converted to an annual dose using the ERB1B dose conversion model) at the location of the hypothetical biosphere (zone 2 shown in Figure 2) are analyzed. The simulations are run for 1 million year in deterministic mode. A subset of radionuclides is included in the calculations to evaluate different radionuclide transport processes. Mean annual doses for the highest dose rate species are shown in Figure 4. The ^{129}I mean annual dose (the highest dose turquoise color line in Figure 4) is the dominant contributor to the dose rate. The long half-life, high solubility, and weak sorption in the far field of ^{129}I contribute to its high mean dose. ^{36}Cl shows as the second highest mean annual dose species, followed by ^{79}Se towards the end of the 1 million year simulation time period.

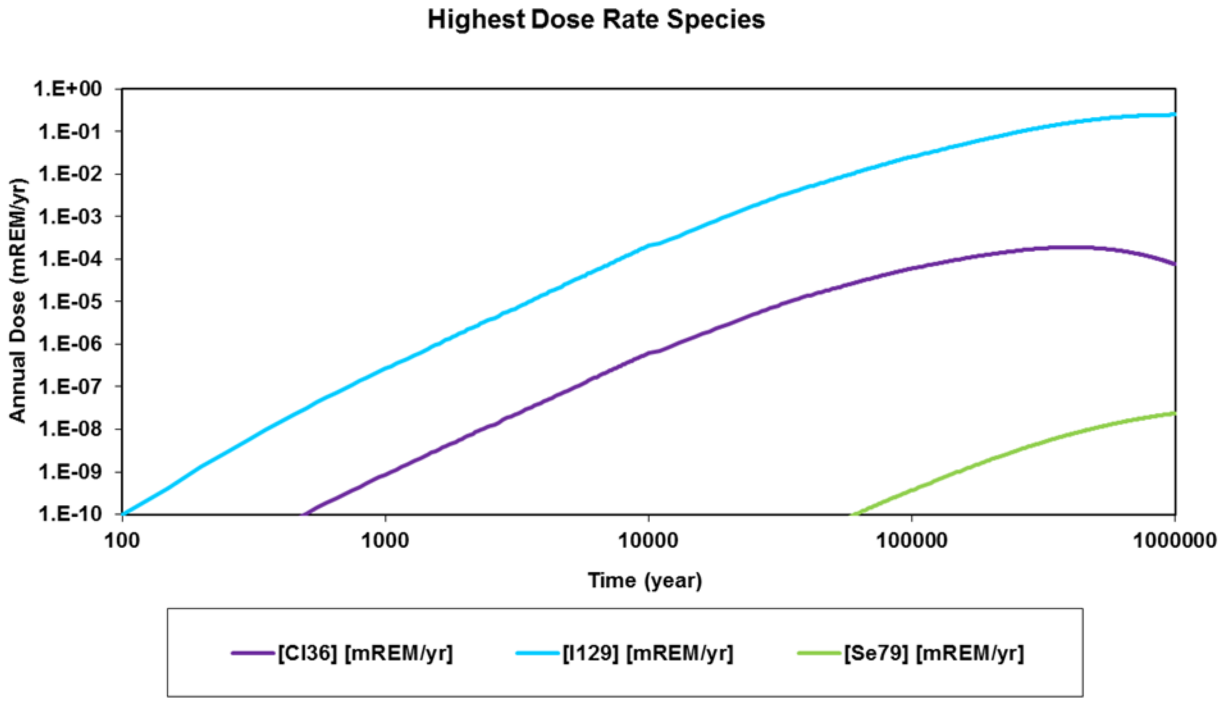

Figure 4. Generic granite system model undisturbed scenario: mean annual dose for individual radionuclide species.
The highest dose rate radionuclide species shown in the order from high to low are ^{129}I, ^{36}Cl, and ^{79}Se.

5. Discussion

The generic granite system model performance assessment results presented in this report 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. The parameter ranges and distributions are selected just for the purpose of demonstrating the generic granite system model analysis; in an actual application, many of these parameters would be site-specific. However, the reference case flow configuration in this study is designed to be similar to the flow models anticipated in future repository performance assessments. The study and analysis discussed can be used to identify the important processes that may affect repository performance in a granite environment.

Future work includes further develop reference case and conceptual models for generic disposal in granite environment; improve generic granite system model by incorporating more detailed physical, chemical and hydrological processes (such as: temperature variation, full representation of repository geometry); conduct system-level and subsystem-level analysis; improve generic granite system model to enhance flexibility and integration to address technical issues with minimal changes.

6. References

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