Performance Assessment Modeling of a Generic UNF/HLW Repository in Salt – 14313

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ABSTRACT

This paper describes the development of an enhanced performance assessment (PA) modeling capability and its application to simulate the post-closure performance of a hypothetical deep geologic disposal system (i.e., repository) for used nuclear fuel (UNF) and high-level radioactive waste (HLW) in a generic bedded salt formation. The enhanced PA capability takes advantage of high-performance computing (HPC) environments to enable the direct integration of the relevant multi-physics processes and couplings into the system model where necessary. Deterministic and probabilistic simulations of the couplings between the radionuclide source term, fluid flow, and radionuclide transport processes in the generic salt repository demonstrate the numerical efficacy of the HPC-based PA capability for these types of complex repository problems.

INTRODUCTION

The U.S. Department of Energy Office of Nuclear Energy (DOE-NE), Office of Used Nuclear Fuel Disposition (UFD) is conducting research to enable disposal of UNF and HLW in a variety of geologic media and generic repository concepts. This paper describes the development of an enhanced PA modeling capability and its application to a demonstration problem of a hypothetical repository in a generic bedded salt formation. The enhanced PA capability takes advantage of HPC environments to simulate the important thermal-hydrologic-chemical-mechanical (THCM) multi-physics phenomena and couplings associated with the waste, engineered barrier system (EBS) components, and natural system of a geologic repository. The HPC-based PA modeling capability integrates the following open-source codes (Fig. 1):

- DAKOTA (Design Analysis toolKit for Optimization and Terascale Applications) – Sensitivity analysis, uncertainty quantification, optimization, and calibration capabilities are provided by DAKOTA [1].
- LIME (Lightweight Integrating Multi-Physics Environment) – Non-intrusive numerical coupling of independent multi-physics codes is provided by LIME [2].
- PFLOTRAN – Multi-physics solutions for a radionuclide source term, engineered barrier degradation and EBS evolution, and flow and transport in the EBS and natural system are provided by PFLOTRAN [3, 4]. PFLOTRAN is an open source, non-isothermal multi-phase flow and reactive transport simulator designed to leverage massively-parallel HPC to simulate subsurface earth system processes. Parallelization is achieved through domain decomposition using the Portable Extensible Toolkit for Scientific Computation (PETSc). PFLOTRAN employs a single, unified framework for simulating multi-physics processes on both structured and unstructured grid discretizations.
- Computational Support Codes – Pre- and post-processing functions are supported by existing codes, e.g., Cubit for mesh generation, VisIt for Visualization, and Python for scripting to process output data for analysis.

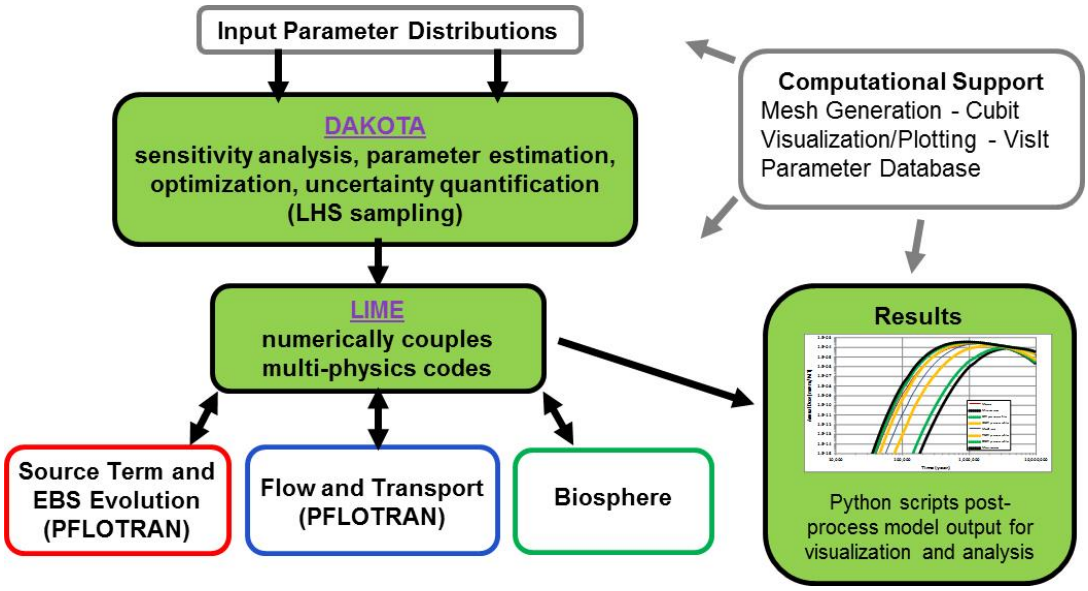


Fig. 1. Code Integration for HPC-based PA Modeling Capability

For the salt repository demonstration problem, PFLOTRAN was used to model source term and EBS evolution as well as flow and transport, as shown in Fig. 1 (Implementation of the radionuclide source term using PFLOTRAN is described in Sec. 2.2.1.4 of Ref. 5). As a result, the multi-physics coupling between these processes was handled within PFLOTRAN, and the LIME code was not required. For a more detailed source term model implemented in an independent code, it is envisioned that the LIME code might be necessary for the coupling.

Salt formations have long been considered a promising host rock for UNF and HLW disposal [6]. For the purpose of demonstrating the enhanced PA modeling capability, a reference modeling case, describing the baseline features and characteristics of a generic salt repository under undisturbed conditions, was developed [5, 7, 8, 9]. Details of the modeling case are documented as part of the salt repository reference case in Sec. 3 of Ref. 5; a summary is presented here.

GENERIC SALT REPOSITORY MODELING CASE

The generic salt repository modeling case consists of an enclosed mode (i.e., waste emplacement with backfilling) disposal concept in a generic bedded salt formation. For the purposes of demonstrating the enhanced PA modeling capability, the modeling case only includes features and processes relevant to an undisturbed scenario. The effects of disturbed scenarios, such as human intrusion, can be examined in future applications. The salt repository modeling case includes a description of the waste region, the EBS components, and the natural system components, including the biosphere (Fig. 2).

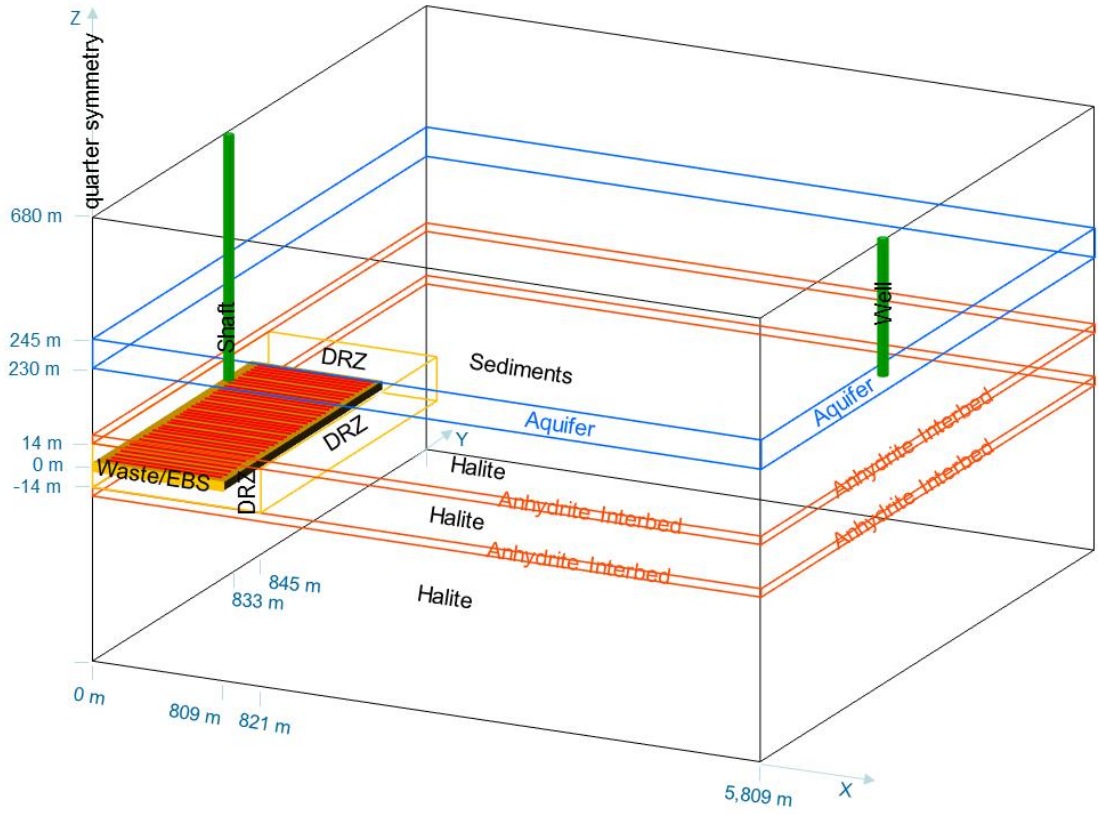


Fig. 2. Generic Bedded Salt Repository Regions

Waste

The waste region implemented in the modeling case includes the radionuclide inventory, waste forms, and waste packages. Details of the waste dimensions and configuration cannot be seen at the scale of Fig. 2.

Inventory and Waste Forms

The modeling case assumes a total repository capacity of 70,000 metric tons of heavy metal (MTHM), consisting entirely of UNF from commercial reactors. The 70,000 MTHM UNF inventory is further simplified to consist entirely of PWR assemblies (uranium oxide (UO_2) matrix with zircaloy cladding). Each PWR assembly is assumed to have characteristics based on current and future PWR discharged through final shutdown of the current reactor fleet in about 2055 [10]. The PWR UNF inventory includes approximately 450 radionuclides (actinides - dominated by ^{238}U, oxygen from the UO_2, zirconium from the cladding, and other fission and activation products) with mass fractions as listed in Table C-1 of Ref. 10. Specific modeling case properties include:

- Each irradiated PWR assembly contains 0.4354 MTHM and a radionuclide composition with a total mass of 1.44 x 10^6 g of radionuclides per MTHM (6.27 x 10^5 g of radionuclides per assembly) and a decay heat of 1.438 kW/MT, based on a 60 GWd/MTHM burn-up, an enrichment of 4.73%, and 30-year out-of-reactor (OoR) decay storage [Table C-1 of Ref. 10].

- Five radionuclides were simulated: the Neptunium series alpha-decay chain (^{241}Am, ^{237}Np, ^{233}U, ^{229}Th) and ^{129}I, a non-sorbing radionuclide with a long half-life. These radionuclides are considered sufficient for the demonstration of the enhanced PA modeling capability because they include radionuclides that are commonly important to long-term dose calculations (^{129}I and ^{237}Np) and a decay chain where daughter ingrowth may be important.
- Only radionuclide releases from UO_2 matrix dissolution are considered. The potential for a fast release fraction from radionuclides located in the fuel and cladding gap and grain boundaries is ignored.
- The waste form matrix dissolution rate is 4.8×10^{-8} mol/m^{3}s (corresponding to 1.5 mol/m^{3}yr), resulting in complete waste form degradation in less than 10,000 years. This rate is much faster than is generally observed under chemically-reducing conditions (e.g., [11]).

Waste Packages

Each waste package is assumed to consist of a stainless steel canister, containing 12 PWR assemblies, and a carbon steel disposal overpack. Limited corrosion of the overpack and canister materials in a typical bedded salt environment may result in waste package integrity being maintained for hundreds or thousands of years [12]. Specific modeling case properties include:

- The 12-PWR loading results in 5.225 MTHM per waste package with an initial thermal output (at 30 years OoR) of 7.5 kW per waste package.
- Approximately 13,400 waste packages are required to accommodate the 70,000 MTHM inventory.
- Each 12-PWR waste package has a length of 5.0 m and an outer diameter of 1.29 m that includes a 5.0-cm thick overpack, corresponding to an outer volume of 6.53 m^3.
- The volume fraction of waste form in a waste package (including the overpack) is 0.104.
- The solid volume of waste, cladding, internals components, and overpack, results in an initial void fraction in a waste package of 0.50. However, to qualitatively account for compaction of the waste package due to salt creep after closure, the modeling case assumes a waste package void fraction of 0.30, which remains constant over the duration of the simulation.
- Each waste package cell was assigned a permeability of 1×10^{-13} m^2, representative of the degraded, compacted waste form and waste package internals.
- Due to the possibility of waste package mechanical damage from salt creep, the modeling case assumes that the waste packages fail instantaneously. As a result, waste package corrosion and associated gas generation is not considered.

Engineered Barrier System (EBS)

The modeling case EBS includes the waste package, drift layout, backfill, and shafts. Based on the modeling case assumption of no gas generation, the EBS is assumed to be brine saturated.

Waste Package and Drift Layout

The modeling case drift layout is based on certain operational, mechanical, and thermal design constraints. The spacing between drifts and the spacing of waste packages within a drift are based on a peak temperature constraint of 200°C at the waste package surface (i.e., at the interface of the waste package with the salt backfill). For the 7.5 kW modeling case waste packages, a spacing of 20 m between drift centers and 10 m between waste package centers in a drift is sufficient to satisfy the thermal constraint [5]. Additional details of the layout include:

- Each excavated emplacement drift is 4 m high, 6 m wide, and 805 m long, with horizontal end-to-end emplacement of waste packages. Drifts are backfilled with crushed salt immediately after waste package emplacement. With 10-m waste package center-to-center spacing, each emplacement drift contains 80 waste packages in an alternating sequence of a 5-m length of backfill and 5-m long waste package.
- Emplacement drifts are laid out in pairs, separated by a 4-m high by 8-m wide central access hallway that connects the drifts. The access hallway will be backfilled upon closure. Each 6-m wide drift pair is separated from adjacent drift pairs in accordance with the 20-m drift center to drift center spacing requirement. The result is a 14-m thick salt pillar between drifts.
- 84 drift pairs (168 drifts) are required to accommodate the 13,400-waste-package inventory.
- The overall repository footprint is 1,618 m (the total length of a drift pair, including the width of the access hallway) by 1,666 m (the total width of the 84 drift pairs and pillars).

Due to the quarter symmetry in Fig. 2, only 42 emplacement drifts (thin red lines in the EBS), each containing 80 waste packages, are shown. These 42 drifts represent one half of 42 drift pairs, the other half of these drift pairs are on the other side of the y-z symmetry boundary.

Shaft

The modeling case includes a stylized shaft that intersects the central access hallway between a drift pair (Fig. 2). The design of the single stylized shaft is based on the four-shaft design from the Waste Isolation Pilot Plant (WIPP) [13]. The stylized shaft is assumed to have a cross-sectional area of 48 m^2 and a total length of 680 m from the ground surface to the depth of the excavated drifts. Shaft seals will be used to isolate the emplacement drifts and to limit water or radionuclide migration through the shafts. The modeling case shaft seal is based on the WIPP shaft seal design. Shaft permeability and porosity values for the modeling case are listed in TABLE I.

Backfill

The crushed salt backfill will begin consolidating as drifts and access hallways close due to creep of the salt host rock. The porosity and permeability of the consolidated backfill is assumed to be the same as for the crushed-salt component of the WIPP shaft seal, which is expected to consolidate to a state close to that of the surrounding intact rock within approximately 200 years [Sec. PA-2.1.3 of Ref. 14]. Backfill permeability and porosity values for the modeling case are listed in TABLE I.

TABLE I. Salt Repository Modeling Case Region Properties

Model Region	**Permeability (m^2)**	**Porosity**	**Effective Diffusion Coefficient (m^2/s)**
Waste Package	1.00×10^{-13}	0.300	6.90×10^{-10}
Backfill	1.00×10^{-18}	0.113	2.60×10^{-10}
Shaft (sealed)	1.58×10^{-20}	0.113	2.60×10^{-10}
DRZ	1.12×10^{-16}	0.0129	2.97×10^{-11}
Halite	3.16×10^{-23}	0.0182	4.19×10^{-11}
Interbed (anhydrite)	1.26×10^{-19}	0.011	2.53×10^{-11}
Aquifer	1.00×10^{-13}	0.200	4.60×10^{-10}

Natural System and Biosphere

The natural system implemented in the modeling case includes the disturbed rock zone (DRZ), the bedded salt stratigraphy (represented by intact halite and anhydrite interbeds), an overlying aquifer, and a pumping well to the biosphere (Fig. 2). All units are assumed to be brine saturated.

Disturbed Rock Zone (DRZ)
The DRZ is the portion of the host rock adjacent to the EBS that experiences durable (but not necessarily permanent) changes due to the presence of the repository. The DRZ tends to be more disturbed early in the postclosure period when thermal and excavation effects are greatest. At later times, healing tends to restore the DRZ closer to ambient conditions (i.e., similar to the intact halite). For the modeling case, the extent of the DRZ is assumed to be 3 drift diameters (i.e., 12 m) and surrounds all sides of the excavation. DRZ permeability and porosity values for the modeling case are listed in TABLE I.

Halite
The host rock halite units are assumed to be relatively pure, intact halite. The modeling case includes a 28-m-thick intact halite unit vertically centered at the repository horizon (i.e., at a depth of 680 m) and additional thicker intact halite units above and below the anhydrite interbeds (Fig. 2). Halite permeability and porosity values for the modeling case are listed in TABLE I.

Anhydrite Interbed
Interbeds are more permeable than the surrounding halite and may become fractured as a result of repository excavation and/or gas generation. The modeling case includes two 1-m thick anhydrite interbeds, one immediately above the DRZ and one immediately below the DRZ (Fig. 2). Interbed permeability and porosity values for the modeling case are listed in TABLE I.

Aquifer
The modeling case includes a 15-m thick aquifer above the repository system (Fig. 2), that may provide a potential pathway (directly or through a withdrawal well) to the biosphere. The aquifer is assumed to have the properties of dolomite, which is a common water-producing unit in bedded salt formations. Flow in the aquifer is driven by a regional hydraulic gradient of 0.001. Aquifer permeability and porosity values for the modeling case are listed in TABLE I.

Biosphere
For the modeling case, a pumping well located 5,000 m from the edge of the emplacement drifts is assumed to provide a pathway to a receptor at the surface biosphere (Fig. 2). However, an explicit biosphere model (i.e., biosphere transport, receptor uptake, and dose calculations) is not included in the demonstration problem. Instead, dissolved radionuclide concentrations calculated at a groundwater sample well location in the aquifer (at a distance of 4,900 m from the $x = 0$ model boundary) are used as a surrogate repository performance indicator for dose.

Thermal and Chemical Environment
The temperature, fluid saturation, and fluid (brine) composition in the EBS and natural system are important because they control the degradation of the waste form and EBS components and the subsequent release and transport of radionuclides. For the modeling case waste package design and layout, in-drift temperatures should be below 100°C after about 600 years, declining to the

far-field ambient temperature of 25°C. The modeling case assumption is that near-field brine exists under chemically reducing conditions after this approximately 600-year thermal period. The far-field brine, which is less affected by temperature, is also assumed to exist under chemically reducing conditions. For the modeling case, the host rock brine composition is assumed to be that of Michigan Basin Devonian Brine because it generally lies within the range of brines from other representative bedded salt formations (Sec. 3.2.3.2 of Ref. 7). The chemical environment influences radionuclide transport through its effect on solubility, sorption, and diffusion.

- Solubility limits – The concentrations of radionuclides dissolved in the aqueous phase may be limited by elemental solubility. At aqueous dissolved concentrations above the solubility limits, radionuclides precipitate to a solid phase. Solubility calculations must account for fractional contributions of all isotopes of the same element. Elemental solubility limits are a function of various radionuclide and fluid (brine) properties such as temperature and pH. The implementation of solubility limits in PFLOTRAN is described in Sec. 2.2.1.4.1 of Ref. 5. Solubility limits for the modeling case elements in a salt repository are listed in TABLE II.

- Sorption – For the modeling case, sorption is assumed to be represented by a linear isotherm, quantified by a distribution coefficient, K_d. Elemental K_d values are a function of various radionuclide, fluid (brine), and rock properties. The implementation of K_d values for sorption in PFLOTRAN is described in Sec. 3.2.3.6.3 of Ref. 5. K_d values for sorption onto salt units for the modeling case elements are listed in TABLE II. The K_d values are for sorption onto anhydrite, but are assumed to apply to all model regions.

TABLE II. Solubility Limits and Distribution Coefficients (K_d) for the Modeling Case

Element	Solubility Limit (mol/L)	K_d (mL/g)
U	1.12×10^{-7}	0.6
Np	1.51×10^{-9}	5.5
Am	5.85×10^{-7}	62.5
I	Unlimited	0.0
Th	4.00×10^{-3}	550.0

- Diffusion – Due to the low salt unit permeabilities for the modeling case (TABLE I), diffusion is expected to be the dominant transport mechanism. The relative importance of diffusive flux through various units is indicated by the effective diffusion coefficient, which is a function of porosity, tortuosity, and the free water diffusion coefficient. For the modeling case, the free water diffusion coefficient is assumed to be 2.30×10^{-9} m^2/s and tortuosity is conservatively (to maximize diffusion) assumed to be 1.0 in all units. Effective diffusion coefficients are shown in TABLE I.

MODEL IMPLEMENTATION

The implementation of the salt repository modeling case includes a single 805-m-long drift containing 80 waste packages. The bottom of the model domain is a horizontal (x-y plane) symmetry boundary imposed through the vertical center of the EBS (i.e., at elevation 0 m in Fig. 2), and the top of the model domain is the top of the aquifer (i.e., at elevation 245 m in Fig. 2).

Appropriate flow and solute transport boundary conditions were applied [5]. The resulting three-dimensional model domain is 5,809 m long (242 grid cells) in the x-direction, 20 m wide (5 grid cells) in the y-direction, and 245 m high (38 grid cells) in the z-direction, as shown in Fig. 3.

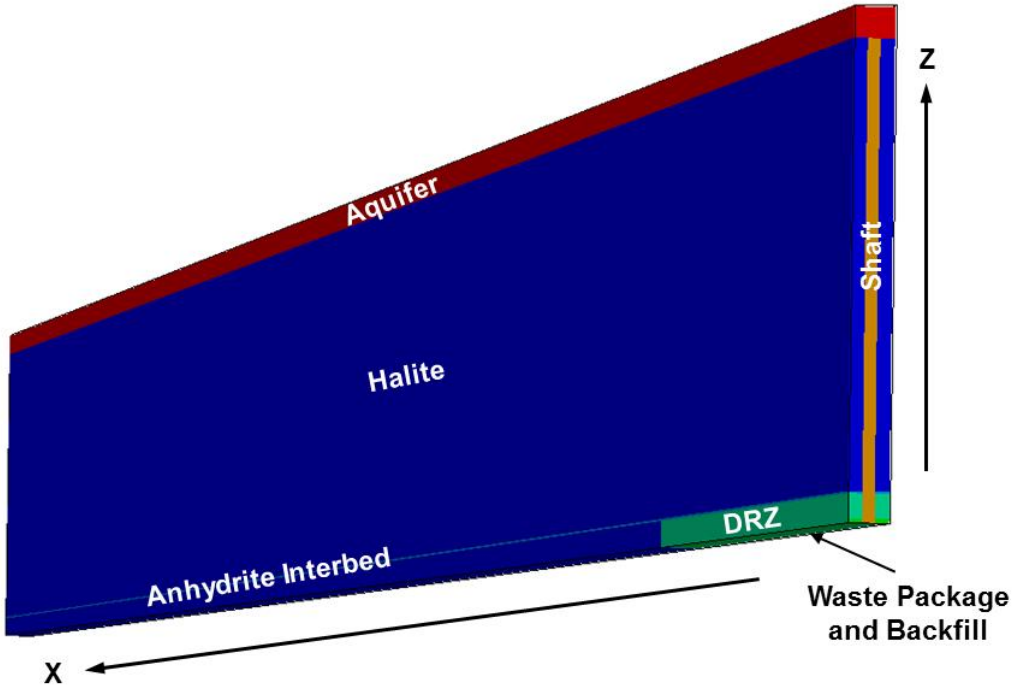


Fig. 3. Salt Repository Modeling Case Model Domain

The HPC-based enhanced PA modeling capability was applied to perform a baseline deterministic simulation and a set of 100 probabilistic simulations for sensitivity analysis. The PFLOTRAN-based multi-physics included representations of the coupled processes of waste degradation, radionuclide mobilization, fluid flow, and radionuclide transport (advection, dispersion, diffusion, sorption, and radionuclide decay and ingrowth) through the EBS and the bedded salt formation to a pumping well location in the aquifer.

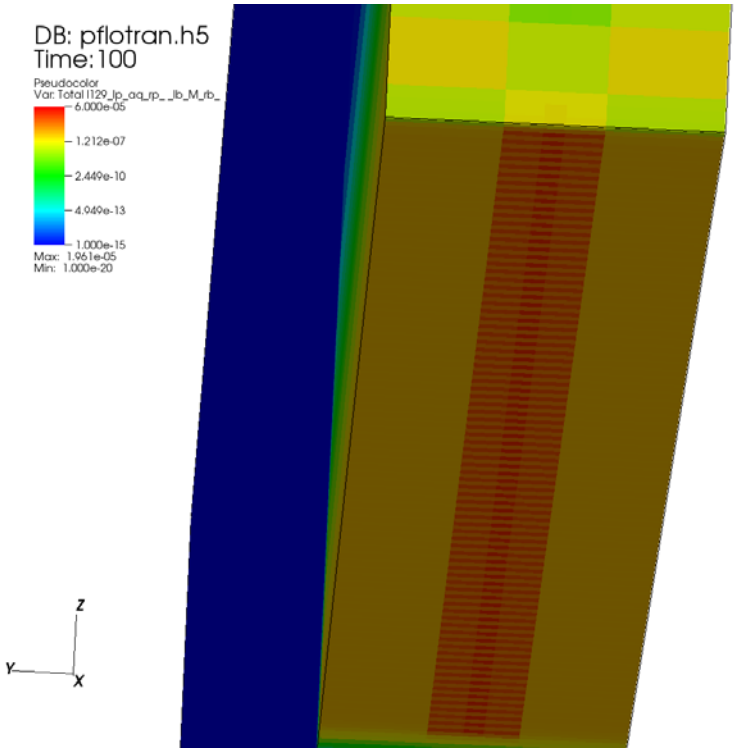
The salt repository demonstration simulations were single phase, isothermal using the PFLOTRAN “Richards” mode; governing equations are documented in Sec. 2 and 3 of Ref. 4. The simulations were performed on the Red Sky high-performance cluster at Sandia National Laboratories. Execution times for a simulation with 413,820 degrees of freedom (45,980 cells tracking 5 radionuclides, 1 primary mineral, and 3 secondary mineral phases) for 1,000,000 years ranged between 0.5 and 3 hours, depending on the number of processors and the parameter values. For the probabilistic simulations, ten concurrent simulations each using 40 processors were run utilizing 800 cores for a total probabilistic run time (i.e., for all 100 realizations) of less than 5 hours. This indicates an average run time of about 0.5 hours for a single simulation on 40 processors. These execution times indicate that reasonably complex probabilistic three-dimensional PA calculations can be performed in acceptable wall clock times.

MODEL RESULTS

The simulations described in this section represent an initial demonstration of the enhanced salt repository PA modeling capability. While the results are based on representative material properties, they are not intended to be used to evaluate the potential performance of an actual bedded salt repository.

Deterministic Baseline Simulation Results

The deterministic simulations were run using “best estimate” modeling case parameter values as summarized in TABLE I and TABLE II. These modeling case parameter values result in diffusion-dominated radionuclide transport through all regions except for the aquifer. ^{129}I is the most mobile radionuclide because it has unlimited solubility and is non-sorbing (i.e., K_d = 0 mL/g). Results from the deterministic simulation are shown in the form of ^{129}I dissolved concentration (reported as molality, i.e., mol/kg solvent) as a function of time and space (Figs. 4 and 5).



(bottom view)

Fig. 4. ^{129}I Dissolved Concentration for the Salt Repository Modeling Case (t=100 years)

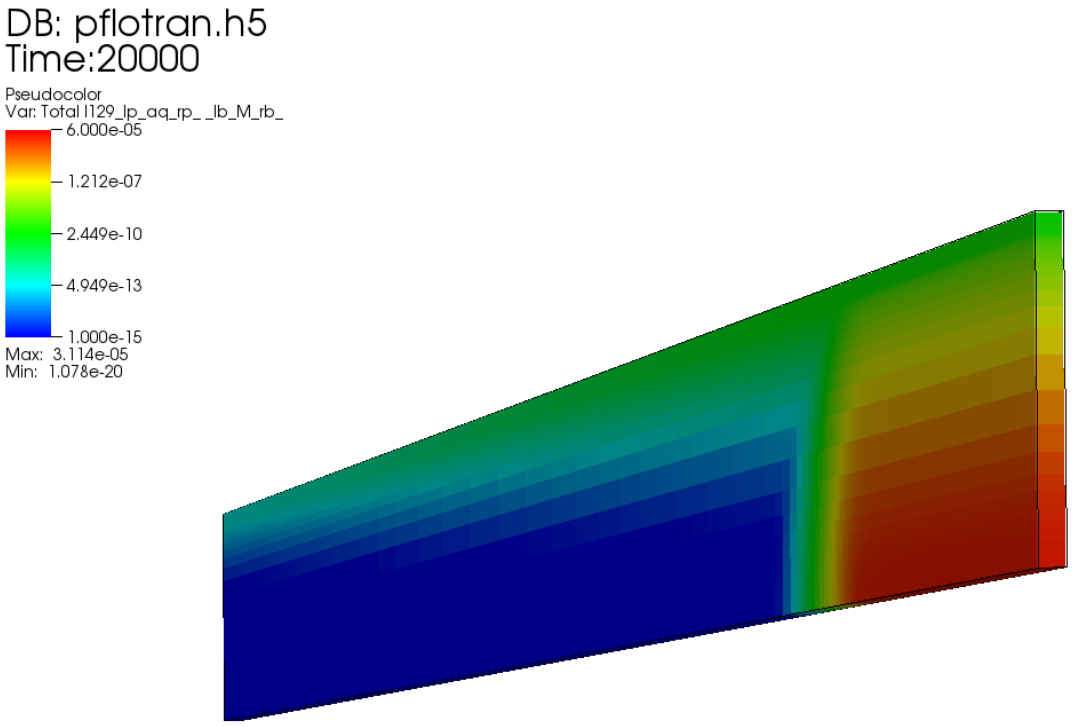


Fig. 5. ^{129}I Dissolved Concentration for the Salt Repository Modeling Case (t=20,000 years)

The waste form begins to dissolve immediately, releasing radionuclides into solution. Fig. 4 is a bottom view of the model domain, showing high ^{129}I dissolved concentrations in the waste and backfill cells after 100 years. Fig. 4 also shows the explicit discretization of 80 individual waste packages in the demonstration problem. Note that the bottom view in Fig. 4 is rotated from the orientation of the side view shown in Fig. 3, and shows the bottom corner of the model domain nearest the edge where the waste and shaft are located.

By 10,000 years, the waste form has completely degraded. ^{129}I released during waste form degradation results in high dissolved concentrations at early times in the waste package and backfill regions, which subsequently diffuses into the DRZ and halite. For radionuclides with solubility limits, secondary mineral volume fractions (i.e., precipitates) increase in the waste package cells. At about 10,000 years, the ^{129}I dissolved concentrations in the aquifer begin to exceed the background level. After about 20,000 years, ^{129}I has been transported by advection down the length of the aquifer and is beginning to diffuse downward into the underlying halite, increasing the concentration in the halite over the entire domain (Fig. 5). This process continues through the duration of the simulation.

Probabilistic Sensitivity Simulation Results

Probabilistic simulations of the salt repository demonstration problem were carried out to further examine the enhanced PA modeling capabilities. One hundred realizations were run with

parameter sampling (using Latin Hypercube Sampling (LHS)) and sensitivity analyses performed using DAKOTA. The nine parameters selected for sampling are shown in TABLE III. Probabilistic results are summarized with a "horsetail" plot of ^{129}I dissolved concentrations at the groundwater sample well location (Fig. 6) and partial rank correlations (Fig. 7).

TABLE III. Salt Repository Modeling Case Probabilistic Parameters

Model Parameter	Deterministic Value	Probability Range	Distribution Type
Waste Degradation Rate (mol/m^{2}s)	4.8×10^{-8}	1.0×10^{-12} - 1.0×10^{-8}	Log uniform
^{129}I K_d (mL/g)	0.00	0.00 – 0.01	Log uniform
Waste Package Porosity	0.30	0.05 – 0.50	Uniform
Backfill Porosity	0.113	0.010 – 0.200	Uniform
Shaft Porosity	0.113	0.010 – 0.200	Uniform
DRZ Porosity	0.0129	0.0010 – 0.1000	Uniform
Halite Porosity	0.0182	0.0010 – 0.0519	Uniform
Interbed Permeability (m^2)	1.26×10^{-19}	1.00×10^{-21} - 1.00×10^{-17}	Log uniform
Aquifer Permeability (m^2)	1.00×10^{-13}	1.00×10^{-14} - 1.00×10^{-12}	Log uniform

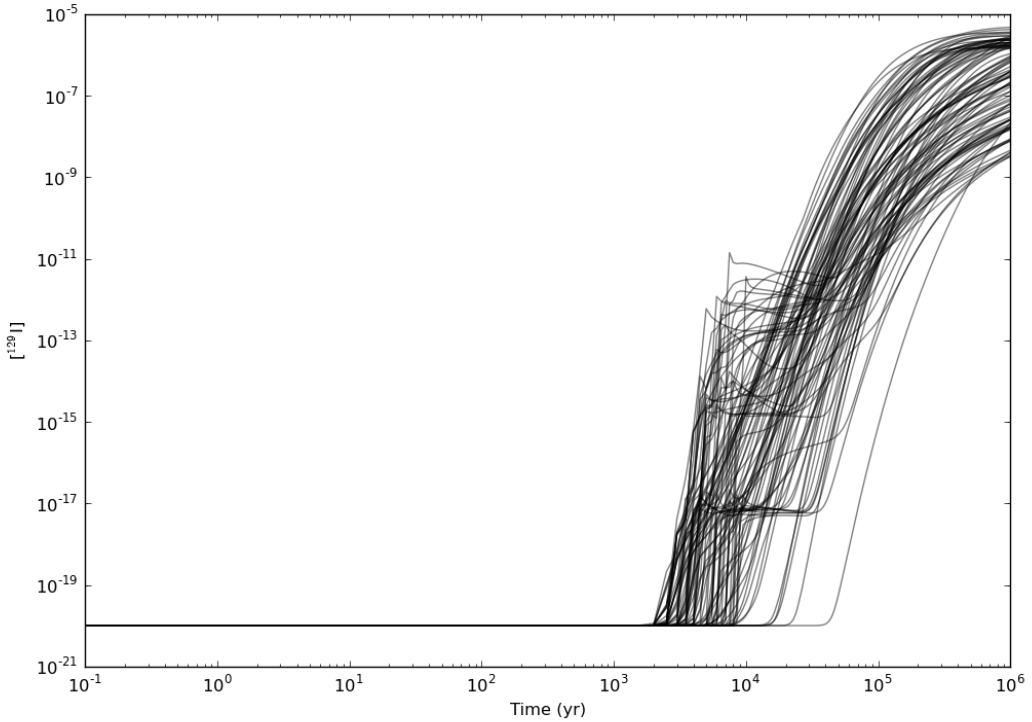


Fig. 6. Horsetail Plot of ^{129}I Dissolved Concentration in the Aquifer at x = 4,900 m

The individual breakthrough curves in Fig. 6 suggest that there are two dominant processes controlling radionuclide transport to the sample well location in the aquifer. The first process is three-dimensional diffusion from the waste and backfill through the DRZ, anhydrite, and halite, and subsequent advection in the aquifer. These transport modes, which are also present in the deterministic simulation, produce an ^{129}I dissolved concentration breakthrough curve which starts to monotonically increase after 10^3 to 10^4 years, and reaches a maximum value at about 10^5 or 10^6 years. The second process is only observable in realizations that have significant advection in the anhydrite interbed (i.e., a high sampled interbed permeability). In these realizations, advective transport distributes ^{129}I along the entire length of the interbed, providing an essentially constant boundary condition for upward diffusion into the entire length of the halite. Thus, subsequent ^{129}I diffusion from the halite to the overlying aquifer occurs at about the same time in all parts of the aquifer. These realizations are characterized by a rapid spike in concentration at the sample well location at around 10^4 years; the sawtooth peaks, and subsequent drops, in concentration give the appearance of a numerical artifact. However, the concentration spikes are due to rapid advection of the ^{129}I in the aquifer away from the sample well location that immediately follows the upward diffusion into the aquifer.

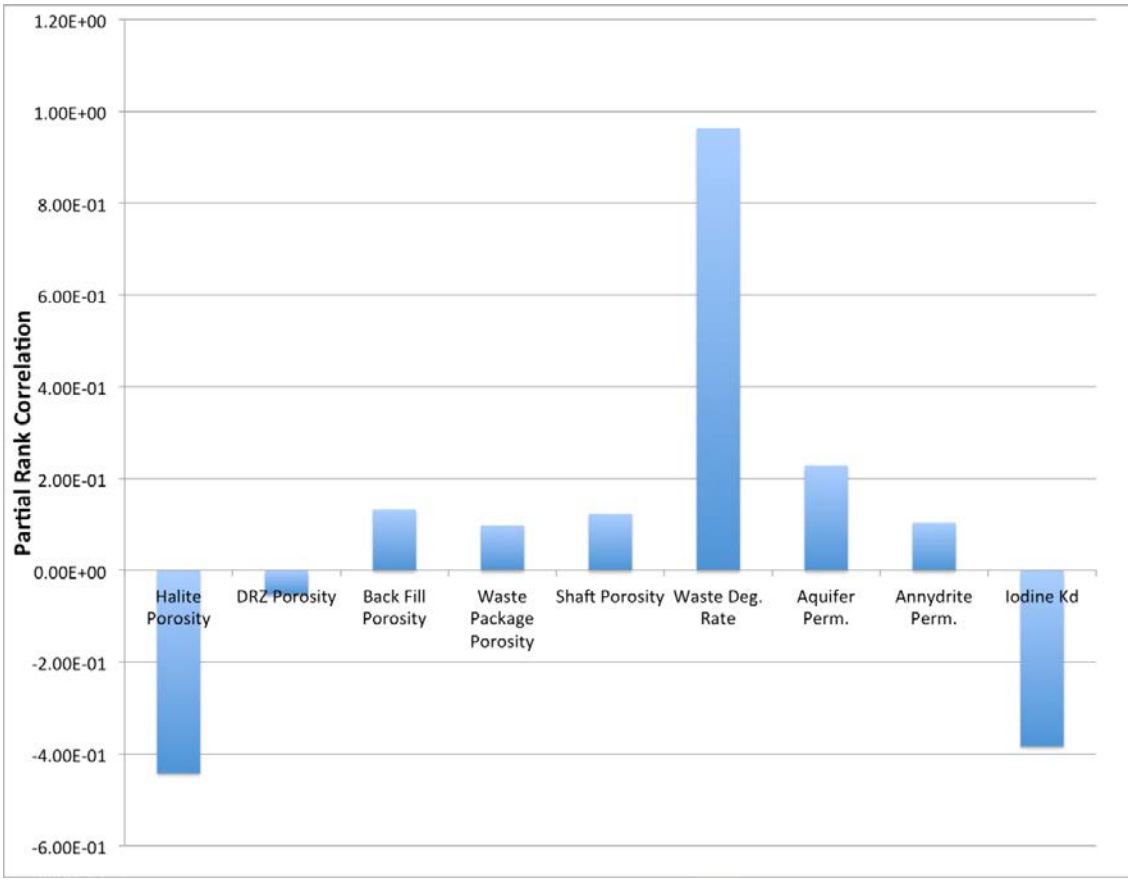


Fig. 7. Partial Rank Correlation of Uncertain Parameters for the Salt Repository Modeling Case

Sensitivity of the performance metric (peak ^{129}I dissolved concentration in the aquifer at the sample well location) to each of the nine uncertain parameters, as quantified by the partial rank correlation, is shown in Fig. 7. The most sensitive parameter is the waste form degradation rate, which contols the source concentration for diffusion. Other sensitive parameters are halite porosity, ^{129}I K_d, and aquifer permeability. The low partial rank correlations for the other five parameters are statistically insignificant.

It is important to note that the sensitivity indicators are dependent on the performance metric, in this case peak ^{129}I dissolved concentration at the sample well location. For example, the high sensitivity to waste form degradation rate would probably diminish if performance metric was total mass transported to the sample well location. Similarly, the sensitivity to ^{129}I K_d would likely be even greater if the performance metric was time to peak concentration.

CONCLUSIONS

A high-performance-computing-based enhanced PA modeling capability was demonstrated by application to a generic bedded salt repository. The results of the deterministic and probabilistic simulations provide insights into the important multi-physics processes and couplings controlling long-term performance for a generic UNF/HLW repository in salt. These insights can be used to guide future research.

The HPC environment enabled reasonable run times for 100 probabilistic simulations of the coupled set of radionuclide source term and flow and transport equations. The application of HPC solutions to the modeling of these coupled phenomena is a significant advancement in PA modeling capability because it allows the important multi-physics couplings to be represented directly, rather than through simplified abstractions.

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