Enhanced Performance Assessment Models for Generic Deep Geologic Repositories for High-Level Waste and Spent Nuclear Fuel – 16223

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ABSTRACT

Development of an enhanced performance assessment (PA) capability for geologic disposal of spent nuclear fuel and high-level waste has been ongoing for several years in the U.S. repository program. The new Generic Disposal System Analysis (GDSA) modeling and software framework is intended to be flexible enough to evolve through the various phases of repository activities, beginning with generic PA activities in the current Concept Evaluation phase to site-specific PA modeling in the Repository Development phase. The GDSA Framework utilizes modern software and hardware capabilities by being based on open-source software architecture and being configured to run in a massively parallel, high-performance computing (HPC) environment.   It consists of two main components, the open-source Dakota uncertainty sampling and analysis software and the PFLOTRAN reactive multi-phase flow and transport simulator.

Reference cases or "generic repositories" have been, and are being developed, based on typical properties for potential salt, clay, and granite host-rock formations and corresponding engineered design concepts for each medium. Past simulations have focused on a generic repository in bedded-salt host rock, while the most recent research has focused on a reference case for a typical clay/shale host rock. A variety of single-realization (i.e., deterministic) and multi-realization (probabilistic) results for the new clay reference case are presented, including an analysis of the effects of heat generation on repository performance, assuming a 100-year out-of-reactor commercial SNF waste form. Order-of-magnitude differences between predicted radionuclide concentrations in thermal versus isothermal simulations imply that mechanistic, coupled-process modeling in three-dimensional (3-D) domains can be important for building confidence in post-closure performance assessments.

INTRODUCTION

According to the U.S. DOE's phased, adaptive, and consent-based approach for siting a final repository for disposal of commercial SNF, the licensing phase for a site-specific repository is scheduled for 2042, with construction to begin in 2048 [1]. Throughout the approximately 30-year timeframe between now and then, it is expected that conceptual models, numerical models, computer hardware, and computer software will all evolve significantly, as indicated schematically in Fig. 1. This evolution from generic performance assessment (PA) during the Concept

Evaluation Phase (currently) to site-specific performance assessment (after final site selection) demands that total system performance assessment models be flexible enough to accommodate concomitant software and hardware evolution. This is an important motivating factor for DOE's current effort to build an enhanced PA modeling capability based on the most advanced hardware architecture currently available, i.e., a high performance computing (HPC), parallel computational environment. It is similarly the motivation for developing the associated PA software in an open-source format. This philosophy embraces the two main goals of the enhanced PA capability, which are to enhance confidence and transparency in the disposal system safety case and to enable better decisions during all phases of repository development, accounting for all relevant technical, political, and fiscal issues and constraints.
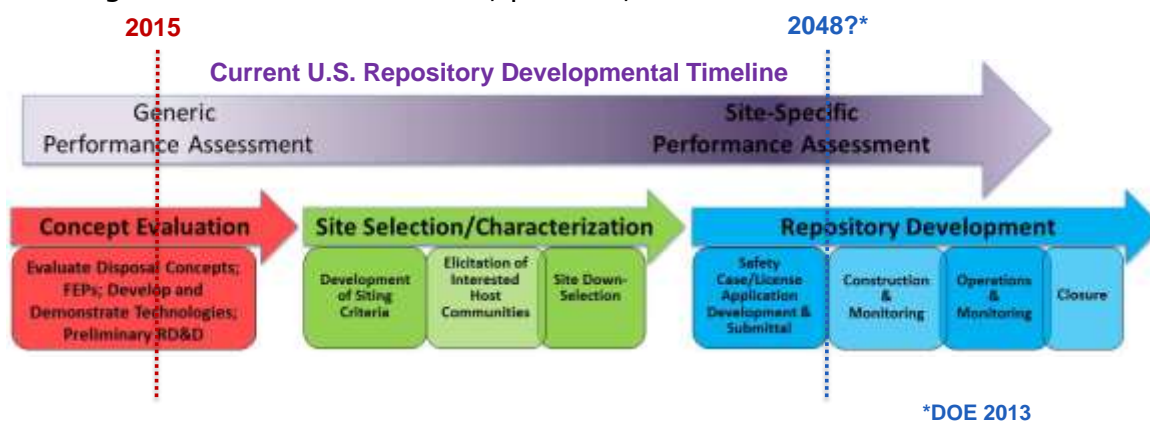

Fig. 1. Developmental timeline for a geologic repository and the associated performance assessment capability.

GDSA MODEL AND CODE ARCHITECTURE

During the evolution from the generic PAs being conducted today to later site-specific PAs, the associated PA model framework has three primary, ongoing functions [2]:

1. Support safety case development during all phases of the disposal system lifecycle

2. Help prioritize *generic* R&D activities (later, *site-specific*)

3. Evaluate potential disposal concepts and sites in various host rock media, and later the chosen site to be licensed

The first function of the enhanced PA model, i.e., support for the repository safety case [3], is facilitated by achieving a more accurate solution to the coupled continuum field equations (mass, momentum, energy) over a large heterogeneous 3-D domain. Two aspects of the enhanced model are necessary in this regard: (1) less reliance on assumptions, simplifications, and process abstractions, i.e., more direct representation of multi-physics couplings in three dimensions within the PA model; and (2) a numerical solution and code architecture that can evolve throughout the repository lifecycle and is able from the outset to use the most advanced hardware and numerical solvers available. Overlying these capabilities is the necessity for

quantification and propagation of uncertainties, both aleatory and epistemic, from input to output.

In consideration of the above, the enhanced PA computational framework, or Generic Disposal System Analysis (GDSA) Framework, consists of the following components:

- Input parameter database

- Software for sampling, sensitivity analysis, and uncertainty quantification (Dakota)

- Petascale reactive multiphase flow and transport code (PFLOTRAN), working in concert with coupled process model codes

- Open-source computational support software and scripts for meshing, processing, and visualizing results (e.g., CUBIT, Python, ParaView, VisIt).

The flow of data and calculations through these components is illustrated in Fig. 2. In a probabilistic simulation, Dakota generates stochastic input for each PA realization based on parameter uncertainty distributions defined in the input set. The sampled inputs are used by PFLOTRAN and its coupled process models to simulate source term release, engineered barrier system (EBS) evolution, flow and transport through the EBS and natural barrier system (NBS), and uptake in the biosphere. After the simulation, various software packages may be used to analyze and illustrate the output calculations of parameters and performance metrics. Dakota may also be used to evaluate the effects of parameter uncertainty on specific outputs.
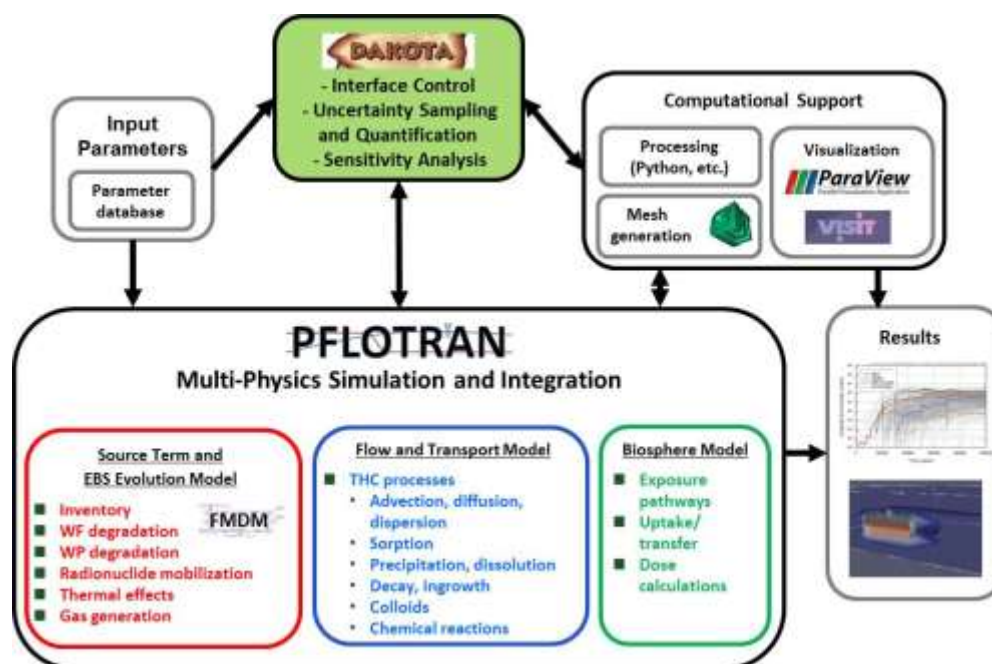

Fig. 2. Generic Disposal System Analysis (GDSA) Framework.

The Dakota software toolkit is open-source software developed and supported at Sandia National Laboratories [4, 5]. The Dakota toolkit is intended as a flexible, extensible interface between simulation codes and a variety of iterative systems

analysis methods, including optimization, uncertainty quantification, nonlinear least squares methods, and sensitivity/variance analysis (https://dakota.sandia.gov/content/about). The GDSA PA Framework uses Dakota as the interface between input parameters and PFLOTRAN. Dakota is also used to analyze the effects of uncertainty in GDSA parameter values on repository performance. Specific capabilities important to GDSA include: (1) generic interface to simulations, (2) mixed deterministic/probabilistic sensitivity analysis, (3) uncertainty sampling and propagation, (4) and scalable parallel computations on HPC clusters.

PFLOTRAN [6, 7, 8] is an open source (https://bitbucket.org/pflotran/pflotran-dev), reactive multi-phase flow and transport simulator designed to leverage massively-parallel high-performance computing to simulate subsurface earth system processes. PFLOTRAN has been employed on petascale leadership-class DOE computing resources to simulate thermal-hydrologic-chemical (THC) processes at the Nevada Test Site [9], multi-phase CO_2-H_2O flow for carbon sequestration [10], CO_2 leakage within shallow aquifers [11], and uranium fate and transport at the Hanford 300 Area [12].

PFLOTRAN solves the non-linear partial differential equations describing non-isothermal multi-phase flow, reactive transport, and geomechanics in porous media. Parallelization is achieved through domain decomposition using the Portable Extensible Toolkit for Scientific Computation (PETSc) [13]. PETSc provides a flexible interface to data structures and solvers that facilitate the use of parallel computing. PFLOTRAN is written in Fortran 2003/2008 and leverages state-of-the-art Fortran programming (i.e. Fortran classes, pointers to procedures, etc.) to support its object-oriented design. PFLOTRAN employs a single, unified framework for simulating multi-physics processes on both structured and unstructured grid discretizations (i.e. there is no duplication of the code that calculates multi-physics process model functionals in support of structured and unstructured discretizations). The code requires a small, select set of third-party libraries (e.g., MPI, PETSc, BLAS/LAPACK, HDF5, Metis/Parmetis). Both the unified structured/unstructured framework and the limited number of third-party libraries greatly facilitate usability for the end user.

PFLOTRAN provides "factories" (code that constructs and destroys data structures, linkages, etc.) within which the developer can integrate a custom set of process models and time integrators for simulating surface and subsurface multi-physics processes. The high-level PFLOTRAN workflow is illustrated in Fig. 3. Within the execution step (Fig. 3a), any number of process models can be coupled and run at identical or dissimilar time scales. The "Process Model Coupler" or PMC class enables this flexibility (Fig. 3b). The PMC is a Fortran class that encapsulates a process model (in this case, multiphase flow), providing numerical methods (time integrators and solvers) for solution, and establishes connectivity between process models. Each PMC has two pointers to other process models, one to a peer and the other to a child. The child PMC is continually playing catch up with the parent PMC. In other words, after each parent PMC time step, the child PMC immediately takes as many time steps as necessary to catch up with the parent, whether the child's time step be lock-step (identical duration) or smaller. The child's time step cannot be larger than the parent.

Necessary information (e.g. state and secondary variables) is transferred to the child immediately prior to the child's step and transferred back immediately after the child catches the parent. The peer PMC, on the other hand, can take any number of time steps of any size and synchronizes with the original PMC at select points in time (synchronization points). In between the synchronization points, the peers are unrestricted by each other and information is only transferred between peers at the synchronization point. In the context of synchronization and the parent-child relationship, the time at the end of the parent PMC's time step becomes the synchronization point for the child PMC.
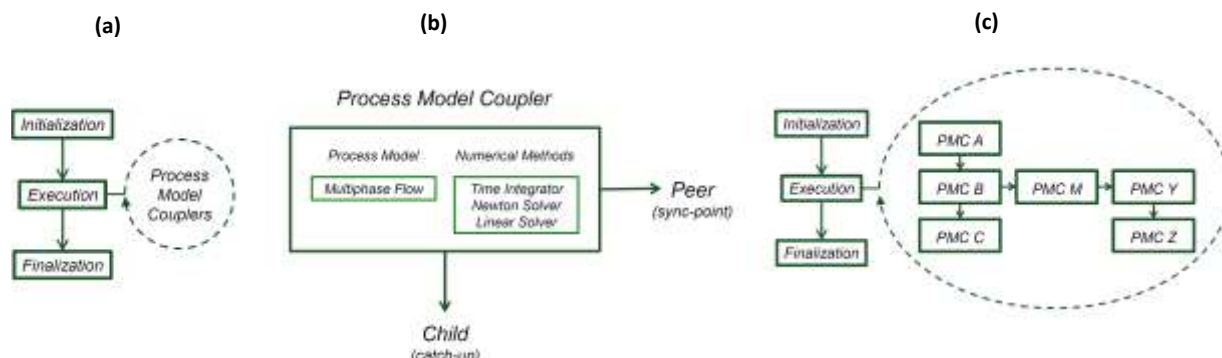

Fig. 3. PFLOTRAN workflow and process modeler couplers: (a) generalized workflow, (b) process model coupler (PMC), and (c) hierarchy of PMCs embedded within the generalized workflow.

PFLOTRAN's PMCs can be nested in sophisticated trees or graphs to accommodate any number of processes coupled across varying time scales. For example, Fig. 3c demonstrates the nesting of six PMCs where PMC A is the parent (and master, meaning it governs all time stepping) with PMCs B, M and Y as its children. PMC A's time step becomes the synchronization point for all three of these children. PMC B and Y also have independent children, C and Z, respectively. A custom factory is built for this simulation that creates the respective PMCs (including underlying data structures, process models, solvers, time integrators, etc.), establishes the hierarchical connectivity, and initializes the PMCs prior to execution and destroys them at shutdown.

APPLICATION OF THE ENHANCED PA MODEL TO AN SNF REPOSITORY IN A GENERIC CLAY/SHALE HOST ROCK

In the current Concept Evaluation phase of repository development (Fig. 1) and associated generic PA, the primary purpose of repository performance simulations is to *demonstrate capabilities* of the enhanced multi-physics HPC performance assessment framework. Radionuclide transport behavior in these idealized simulation domains is a result of the assumed material properties in the various domains of the generic repository and may or may not reflect conditions at the to-be-selected repository site. During this Concept Evaluation phase, generic "reference cases" are used to represent repositories in various host-rock media, based on typical properties for clay/shale, salt, or granite/crystalline host rock in the U.S., along with generic engineered designed concepts that are appropriate for these host rocks.

Various capabilities of the GDSA Framework for a generic repository in bedded salt have been demonstrated elsewhere [2, 14, 15], including a recent comparison between a "quasi 2-D," single-drift pair and a more representative 3-D domain containing five drift pairs [16]. This comparison shows that the combined effect of coupled thermal-hydrologic processes and three-dimensional geometry can affect total system performance predictions in a non-trivial way.[a] Two new generic reference cases include a salt repository reference case for DOE-managed HLW and a clay/shale repository reference case for commercial SNF. This section describes the application of the GDSA Framework to the new generic clay/shale repository. The initial focus of the generic reference cases is still the undisturbed scenario (e.g., performance in the absence of external events) rather than on disturbed scenarios (e.g., human intrusion, seismic activity). This is logical for generic repository analyses because disturbed scenarios are strongly dependent on site-specific information and regulatory considerations, not currently available.

Clay-rich formations are an attractive disposal medium due to their low permeability, high sorption capacity, typically reducing pore waters (which limit radionuclide solubility), and ability to deform plastically (if not indurated), which promotes self-healing of fractures. The U.S. hosts several marine sedimentary sequences containing thick beds of clay-rich sediments potentially suitable for deep geologic disposal of radioactive waste [17, 18]. The clay reference case described here draws upon recent work of Hansen et al. [19], Clayton et al. [20], and Freeze et al. [14] for conceptualization of a mined geologic repository in shale, and Jove-Colon et al. [21] for the details of drift-emplacement and the engineered barrier system.

The generic disposal concept in clay is similar to that in salt. Exact details regarding material properties and configurations of the generic EBS and NBS are given by Mariner et al. [16]. Here, a brief summary must suffice. As in the salt case, waste disposal occurs in a mined repository located in a deep, homogeneous, thickly bedded, low-dip stratum in a geologically stable environment. The repository consists of excavated emplacement drifts laid out in pairs, separated by a central access hallway, and shafts used for construction, operation, and ventilation. Waste packages are emplaced horizontally, end-to-end in each drift. However, the clay reference case differs from the salt reference case in ground support methods, backfill material, and thermal considerations. Whereas a mined repository in salt requires minimal ground support, it is assumed that a mined repository in clay will require cement liners in drifts, hallways, and access shafts to prevent spalling [21]. Similarly to the salt host-rock repository, in which crushed salt is used as backfill around the waste packages, waste packages in the generic clay host-rock repository are surrounded with a bentonite clay buffer/backfill, which acts as a low permeability seal to prevent radionuclide transport away from breached waste packages.

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[a] For example, thermally driven fluid convection cells established in a narrow 3-D domain ("quasi 2D") are not apparent in a wider multi-drift 3-D domain where heat is dissipated laterally. This can affect radionuclide transport until the decay heat pulse dissipates several tens of thousands of years after repository closure.

Disposal in clay/shale repository concept presents greater thermal challenges than disposal in salt due to the much lower thermal conductivity of clay/bentonite, which will heat the waste package to a much higher temperature than in the salt host-rock case, assuming the same waste-package loading (i.e., number and heat generation rate of fuel rods in a waste package) and emplacement layout. This combined with the issue that near field temperatures above 100°C may alter properties of the bentonite buffer [22, 23] leads to several clay-specific design provisions, including (1) a bentonite/quartz (70%/30%) buffer to increase the buffer thermal conductivity; and (2) decay storage of the SNF for 100 years out of reactor (OoR) [24, Table C-2]. Other possible design changes, not implemented in this study, include a greater drift spacing and/or a greater in-drift waste package spacing, as well as a double-layer concentric buffer [21], where the layer closest to the waste package is a "sacrificial" bentonite/quartz material, while the outer layer is pure bentonite for its sealing/swelling properties.

The waste package is assumed to consist of a stainless steel canister containing 12 PWR SNF assemblies and a carbon steel overpack. The waste package is 5 meters long and has a diameter of 1.29 meters, consistent with the 12-PWR waste package described by Hardin et al. [23]) and identical to that used in the salt case. The clay reference case makes the conservative assumption that all waste packages fail instantly. The nature of the spent fuel inventory in the waste packages is identical to the SNF inventory considered in the salt reference case (i.e., 70,000 MTHM comprised entirely of PWR assemblies with a burnup of 60 GWd/MTHM and initial enrichment of 4.73 wt% ^{235}U), except that in the clay case the spent fuel is aged to 100 years OoR. This assumption is necessary, as described above, to regulate temperature in the repository due to the low thermal conductivity of bentonite and clay/shale. Initial radionuclide inventories for the clay case are given by Mariner et al. [16, Table 4-14] for a set of actinides and fission products used for testing of the GDSA Framework: ^{241}Am, ^{237}Np, ^{233}U, ^{229}Th, ^{242}Pu, ^{238}U, ^{234}U, ^{230}Th, ^{226}Ra, and ^{129}I. Because ^{129}I is the most mobile of these radionuclides, being almost completely nonsorbing with effectively unlimited solubility, it is the nuclide that is focused on here.

The NBS comprises the clay formation hosting the repository, the disturbed rock zone (DRZ) adjacent to the repository, and geological formations above and below the host formation. On the basis of stratigraphic sequences observed in sedimentary basins throughout the U.S. [17, 18], the NBS is conceptualized as a thick (on the order of thousands of meters) marine depositional sequence created by transgression and regression of inland seas, and consisting of thick layers of low permeability sediments such as shales and marls alternating with thinner layers of high permeability sediments such as limestones and sandstones. Specifically, the NBS includes a 500-meter thick shale formation containing a homogeneous repository horizon (Fig. 4a) and two thin (5 meter) high-permeability interbeds (such as limestone) 125 meters above and below the repository horizon; two 50-meter thick sandstone aquifers above and below the 500-meter shale formation; 200 meters of generic (non-lithified) sediments above the upper aquifer; and a 100-meter thick low-permeability confining layer (such as another shale formation) below the lower aquifer. Layer thicknesses and material properties are loosely based on the regional

stratigraphy surrounding the Cretaceous Pierre Shale and Dakota Sandstone (e.g., see [25, 26]), and are consistent with those used in previous models of generic clay repositories [19, 27] and within the range of those found in other marine depositional sequences in the U.S. [17, 18]. The DRZ is conservatively assumed to be a 9-meter thick zone adjacent to the drift walls.

A mined repository in shale is expected to require the support of shotcrete (sprayed concrete). The assumed shotcrete thickness in all excavations (drifts, halls, and shafts) is 0.75 m. Material properties are based on WIPP concrete and the shotcrete described by Jove-Colon et al. [21, Table 12]. The repository layout is similar to that in the salt case. Pairs of disposal drifts lie at right angles to a central access hallway. Drift centers are separated by 20 meters. Waste packages are emplaced horizontally, lengthwise within the drifts with a spacing of 10 meters center-to-center (5 meter spacing, end-to-end). Unlike the salt case, the drifts are assumed to have a circular cross-section with a diameter of 4.5 meters [21]. Detailed repository dimensions are listed by Mariner et al. [16, Table 4-17].

The clay reference case conceptual model assumes a regional setting with no topographic relief, horizontal bedding, a regional geothermal heat flux of 60 mW/m^2 (appropriate for midcontinent U.S. [28]), and a regional head gradient west to east of □0.0013 (m/m), similar to gradients observed in the Cretaceous aquifers of the northern Great Plains [29, 30]. The stratigraphic section is shown schematically in Fig. 4. The repository is placed in the middle of the shale layer, 500 meters below the surface, and 5 kilometers from a hypothetical withdrawal well, at which location radionuclide concentrations are monitored in the overlying aquifer. The model domain is a rectangular prism, 12,653 meters long in the x direction, 5000 meters wide in the y direction, and 900 meters tall in the z direction. The modeled repository consists of 5 drift pairs, a total of 800 waste packages, a central access hallway, and a shaft. Due to the choice of a reflective boundary condition at $y = 0$ m, this domain is equivalent to 10 drift pairs, 1600 waste packages, and 2 shafts centered in a 10,000-meter wide domain.

Processes considered in the clay reference case simulations include convective and conductive heat transport, advective, diffusive, and dispersive solute transport, waste form degradation, mineral precipitation and dissolution, sorption, and radioactive decay and ingrowth.
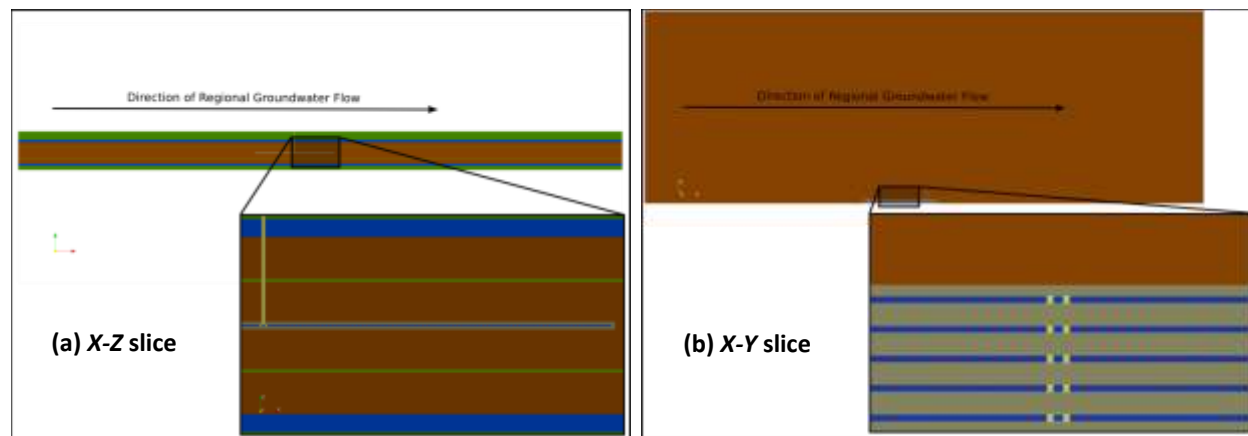
Fig. 4. (a) *X-Z* slice of the clay reference case domain at the *Y* midpoint of the first drift pair and (b) *X-Y* slice at the vertical center point of the drifts. [Clay is shown as dark brown, sediments as dark green, aquifers as royal blue, DRZ as grey, interbeds as bright green, bentonite/quartz buffer as dark blue, and the shaft/seals as yellow.]

Two deterministic cases (i.e., single-realization, "best estimate" properties) are simulated and compared for the generic clay repository to investigate the effects of coupled processes on repository performance: (1) an isothermal simulation in which the effect of decay heat is ignored and (2) a thermal simulation in which heat and fluid flow are treated as coupled processes. In addition, a probabilistic simulation is conducted for the isothermal case, using 50 realizations of nine input parameter uncertainty distributions.

Deterministic Isothermal Simulation

Initial conditions specified for the isothermal simulations are fluid pressure and radionuclide concentrations. Initial pressure throughout the model domain produces a hydrostatic gradient in the vertical direction, and a head gradient of $\square$0.0013 (m/m) from west (left) to east (right). The release and transport of five radionuclides is considered: ^{241}Am, ^{237}Np, ^{233}U, ^{229}Th, and ^{129}I. Initial radionuclide concentrations in all cells except the waste package cells are $10^{\square 20}$ mol/L (an approximation of 0 mol/L on a logarithmic basis). In the waste package cells, initial concentrations of ^{241}Am, ^{237}Np, ^{233}U, and ^{229}Th are set to $10^{\square 20}$ mol/L and initial concentrations of ^{129}I are $7.25 \times 10^{\square 4}$ mol/L to account for the instant release of ^{129}I from the waste form. Boundary conditions must be set for the six faces of the model domain. The west (left), east (right), and back faces are held at initial pressures in order to maintain the west-to-east head gradient throughout the simulation time. Radionuclide concentrations at these faces are held such that any fluid entering the model domain contains $10^{\square 20}$ mol/L of each radionuclide, while fluid exiting the model domain is allowed to carry with it ambient concentrations. Diffusive flux is disallowed at the outlet boundary by specifying a zero concentration gradient. Top, bottom, and front faces of the domain are no-flow boundaries (constant head and concentration gradients of zero).

[129]I concentrations in the model domain at various times are shown in Fig. 5. Because the bentonite shaft seal and the surrounding host-rock shale have similar material properties, preferential diffusion up the shaft does not occur as it does in the salt host-rock case [2]. At early times, while aqueous [129]I is confined to the repository, DRZ, and surrounding shale formation, transport is primarily by diffusion, as can be seen in Figs. 5a and 5b. When [129]I reaches the aquifers above and below the shale, advective transport becomes important and the [129]I plume spreads out in the direction of regional groundwater flow (positive x, or to the east; Figs. 5c and 5d). At 10^6 years (Fig. 5d), the 3-D [129]I concentration contour at the well-observation location ($x = 11,621$ m) is slightly less than $= 5 \times 10^{-11}$ mol/L. This concentration is approximately one order-of-magnitude less than the limit set by the World Health Organization for [129]I in drinking water [31].
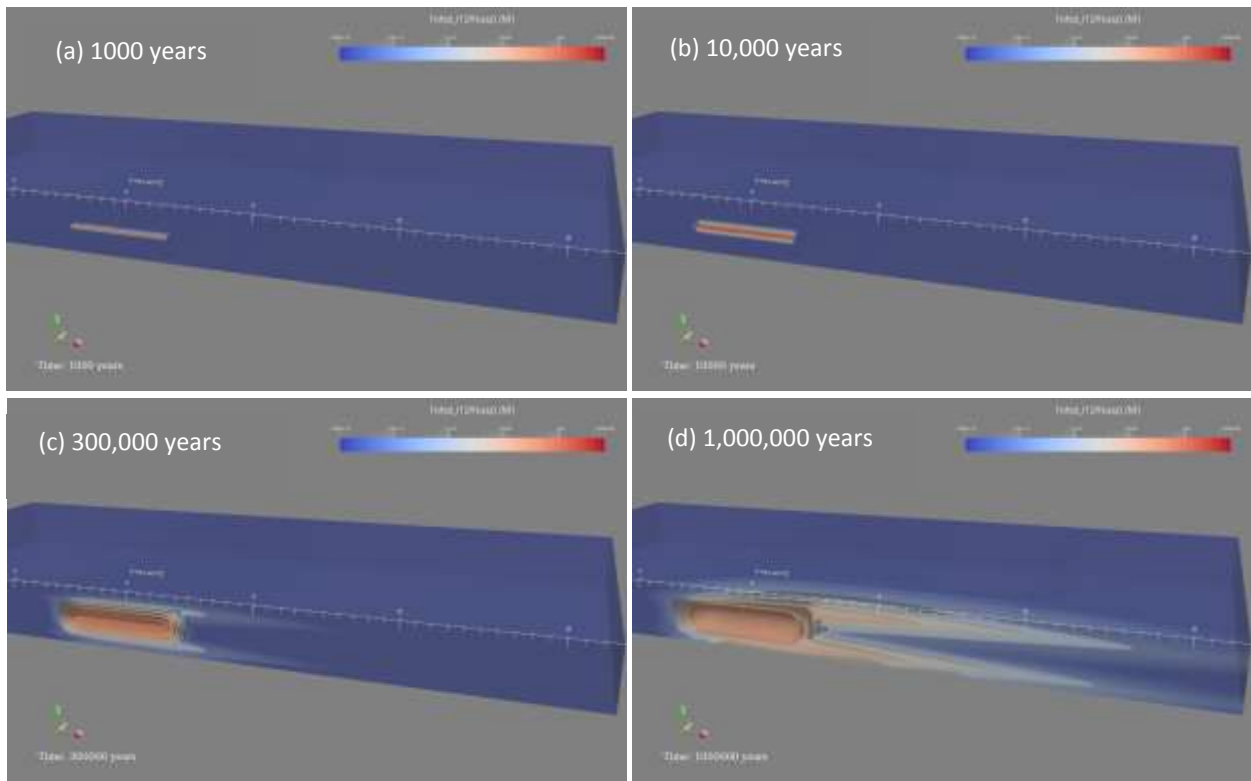

Fig. 5. Dissolved [129]I concentration at specified times for the deterministic isothermal generic clay repository simulation: (a) 1,000 years, (b) 10,000 years, (c) 300,000 years, and (d) 1,000,000 years.

Probabilistic Isothermal Simulation Results

Selected parameters, with the epistemic uncertainty distributions shown in TABLE I, were sampled using Dakota. Radionuclide breakthrough ([129]I) was monitored at 10 observation points, shown in Fig. 6, all of which lie on the midline of the first drift pair ($y = 10$ m).

TABLE I. Clay-repository reference-case probabilistic parameter distributions.

| Model Parameter	Deterministic Value	Probability Range	Distribution Type
Waste form degradation rate constant (mol/m^2/s)	4.8×10^{-8}	$10^{-10} - 10^{-7}$	Log uniform
^{129}I K_d (ml/g)	0.0	$9.28 \times 10^{-7} - 7.84 \times 10^{-3}$	Log uniform
^{237}Np K_d (ml/g)	173	30 – 1000	Log uniform
Bentonite/Quartz Buffer Porosity	0.25	0.1 – 0.4	Uniform
Shaft Porosity	0.4	0.1 – 0.4	Uniform
DRZ Porosity	0.25	0.1 – 0.4	Uniform
Shale Porosity	0.25	0.1 – 0.4	Uniform
Interbed Permeability (m^2)	1.0×10^{-16}	$10^{-18} - 10^{-14}$	Log uniform
Aquifer Permeability (m^2)	3.2×10^{-15}	$10^{-16} - 10^{-13}$	Log uniform
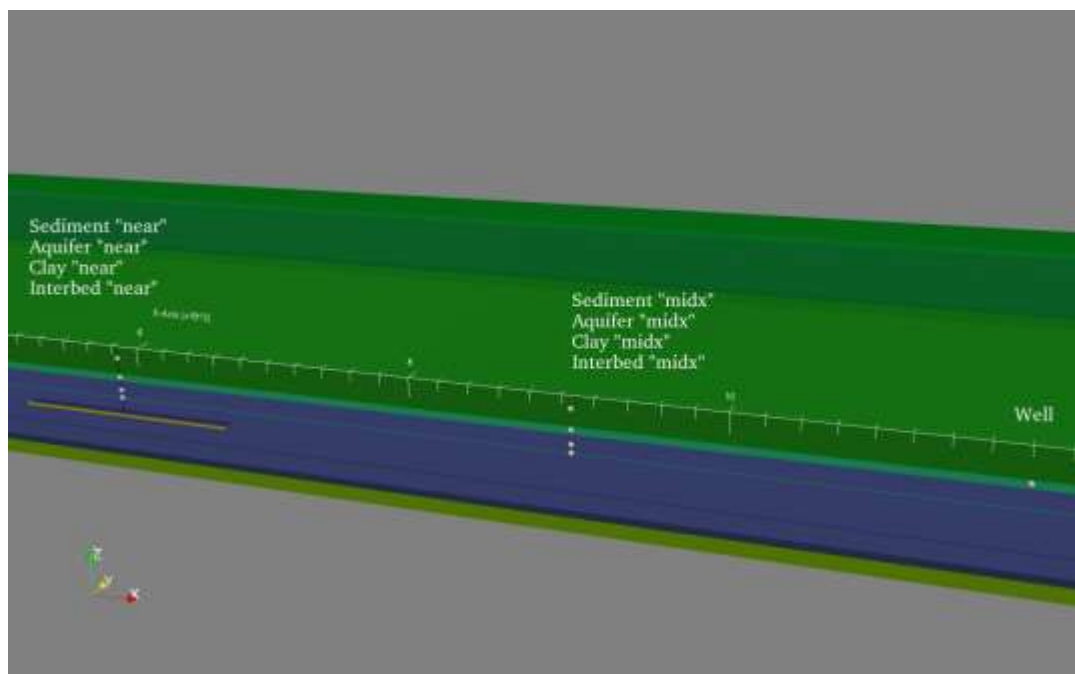
Fig. 6. Locations of observation points for sensitivity analyses of probabilistic simulations. ["Near" observation points are 7 m east of access shaft.]

Fig. 7 shows ^{129}I breakthrough curves for each of the observation points, and Fig. 8 shows Spearman rank correlation coefficients relating maximum dissolved ^{129}I concentration to the sampled parameters at the four "near" observation points. At the two "near" observation points closest to the waste packages (interbed and clay) maximum ^{129}I concentrations vary by only about one order-of-magnitude between realizations (Fig. 7), with the spread being predominately a function of waste form

degradation rate (positive correlation) and shale porosity (negative correlation) (Fig. 8). At other observation points (Fig. 7), the spread in maximum [129]I concentration among realizations (all occurring at 1,000,000 years) is significantly greater because it is a function of more of the uncertain parameters in TABLE I, such as aquifer permeability, and because these observation points are farther from the source, allowing more time for diffusion/dispersion. At the "near" observation points in the aquifer and sediment formations (Fig. 8), there is a strong negative correlation between maximum [129]I concentration and aquifer permeability because the higher the aquifer permeability the greater the fluid flow rate, which causes a greater dilution of the [129]I concentration in the aquifer.
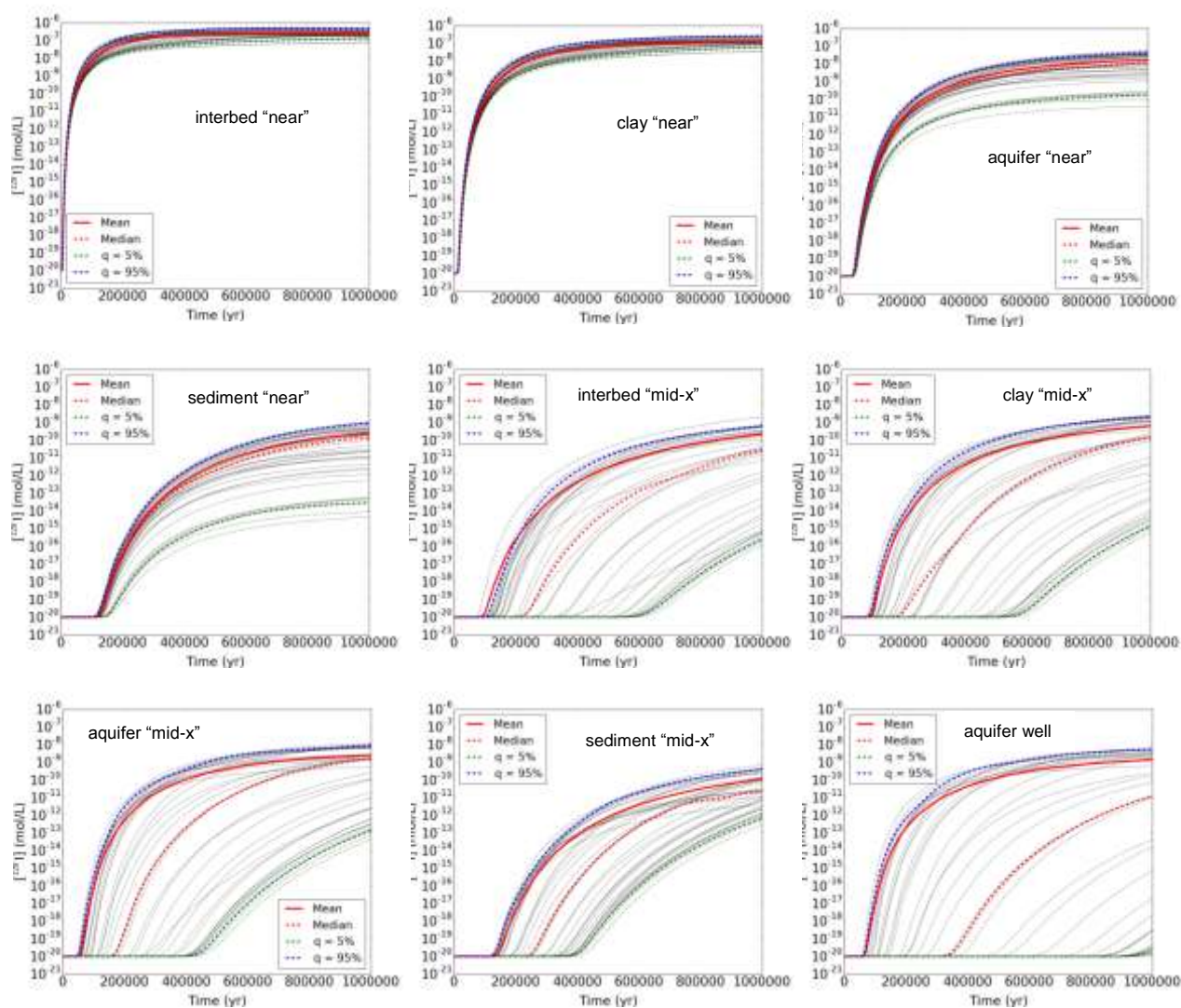

Fig. 7. Multi-realization time histories of dissolved [129]I concentration at various observation points for the probabilistic isothermal generic clay repository simulation.
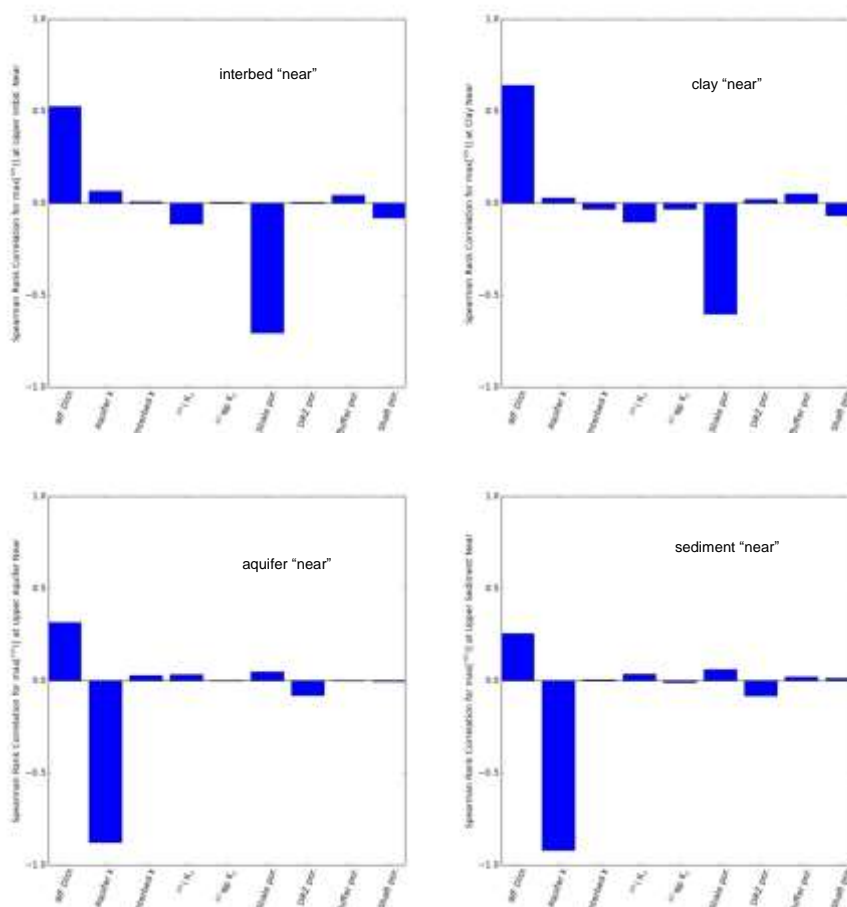
Fig. 8. Spearman rank correlation coefficients for maximum dissolved ^{129}I concentration versus sampled parameters for the probabilistic isothermal generic clay repository simulation at the four "near" observation points.

Deterministic Thermal Simulation Results

Whereas fluid flow in the isothermal simulations is due solely to the imposed regional head gradient, the clay deterministic *thermal* simulation includes coupled heat flow and fluid flow. Heat generated by radioactive decay in the waste form drives fluid flow in and around the repository. Temperatures and flow patterns in the near field at various times are summarized in Fig. 9. At a simulation time of 0 years (prior to repository heating), a background geothermal temperature gradient (generated by a basal heat flux of 60 mW/m^2) and a regional fluid flow field are established. As repository temperatures rise, a corresponding increase in fluid pressure drives fluid flow out of the repository (Fig. 9, at 10 years). Maximum repository temperatures are reached around 100 years but fluid flow continues out of the repository for several thousand years (Fig. 9, at 1000 years). By 10,000 years, fluid pressure in the cooling repository has dropped enough that fluid begins to flow back into the repository. The repository continues to cool and the flow field approaches that due to background head gradients throughout the remainder of the simulation time (Fig. 9, at 100,000

years). However, regional fluid flow is still slightly disturbed by the repository after even 1,000,000 years.
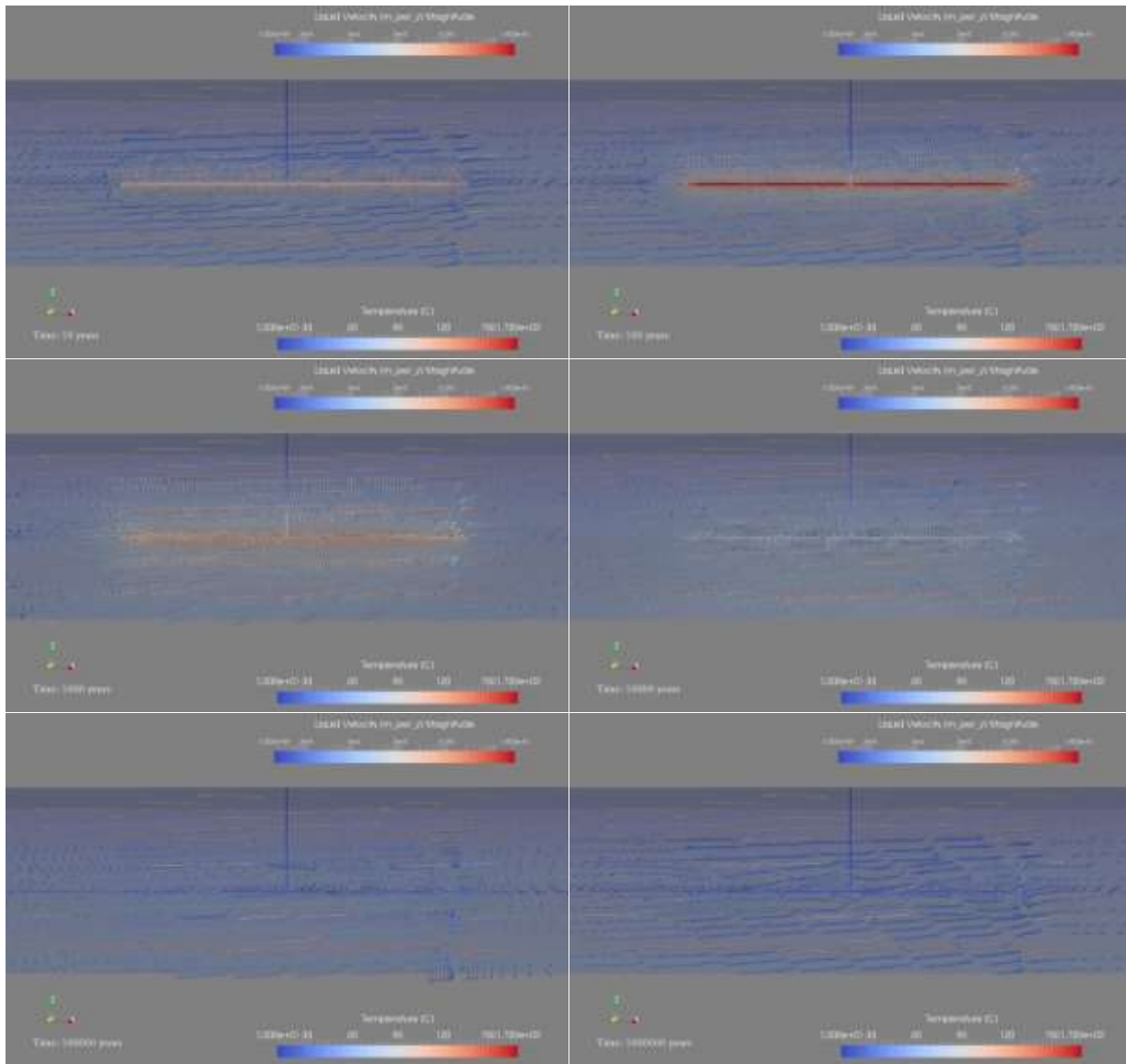

Fig. 9. Near field temperature and Darcy velocity at various times (10; 100; 1,000; 10,000; 100,000; and 1,000,000 years) for the deterministic *thermal* generic clay repository simulation.

In the thermal simulation, the cooling repository has the effect of drawing fluid inward, and therefore inhibits radionuclide transport outward and decreases ^{129}I concentrations in the far field by about an order-of-magnitude compared to concentrations predicted by the isothermal simulation. This difference can be seen by a comparison of ^{129}I breakthrough curves at the well observation location (Fig. 10) and in the 3-D contours of ^{129}I concentration at various times for the thermal simulation (Fig. 11) compared to the isothermal simulation (Fig. 5). In contrast to the isothermal simulation, the thermal simulation predicts that at 10^6 years the 5 ×

10^{-11} mol/L concentration contour will fall approximately one kilometer short of the well observation location (x = 11,621 m). The difference in predicted system behavior brought about by adding the mechanism of coupled heat and fluid flow to the simulation highlights the importance of multi-physics, mechanistic models for obtaining accurate model predictions. Within the constraints of computational feasibility and data availability, mechanistic models should be used whenever possible.
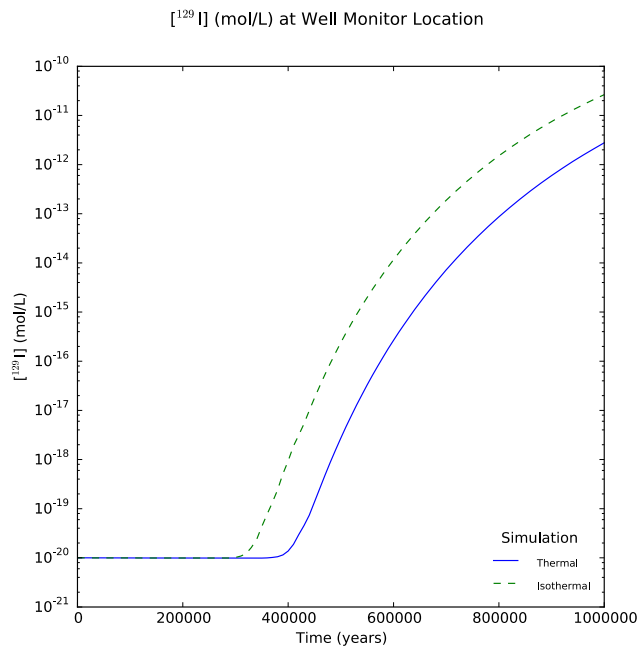

Fig. 10. Comparison of dissolved ^{129}I concentration versus time at the well observation point for the deterministic *thermal* and isothermal generic clay repository simulations.
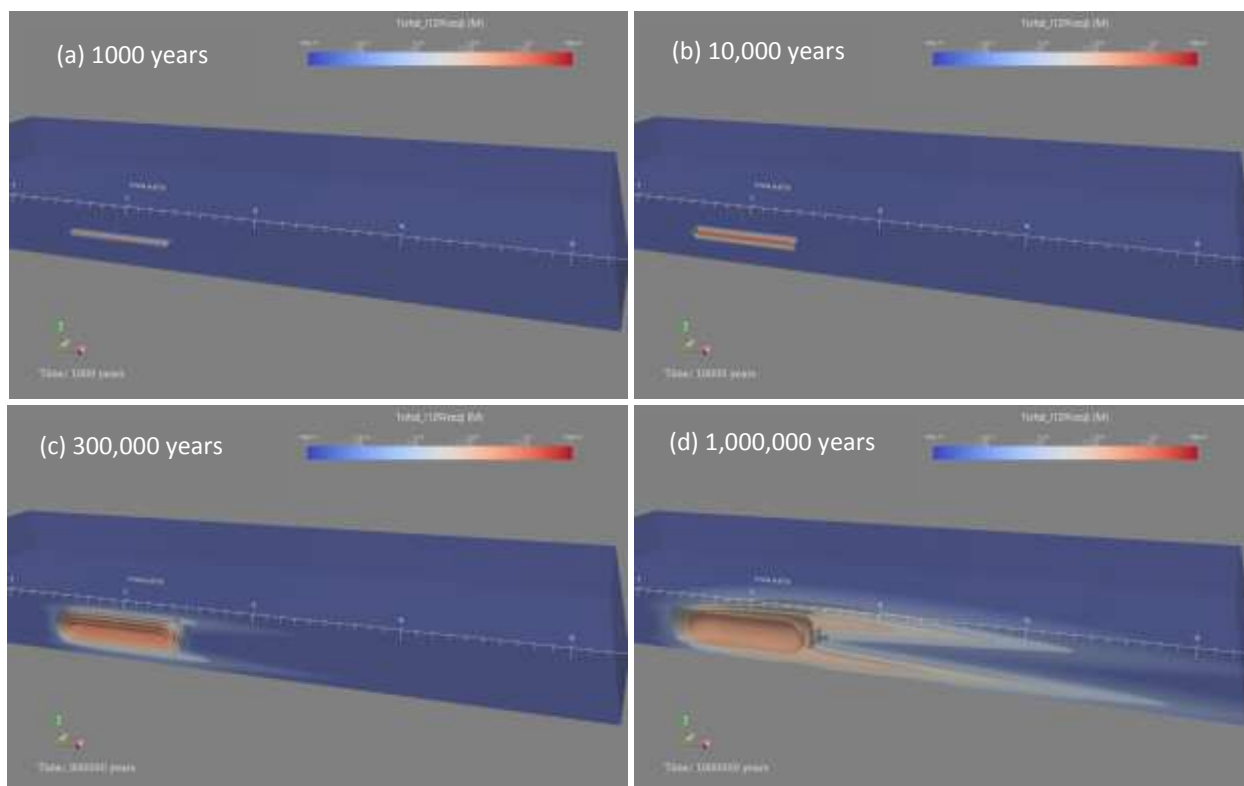
Fig. 11. Dissolved [129]I concentration at specified times for the deterministic *thermal* generic clay repository simulation: (a) 1,000 years, (b) 10,000 years, (c) 300,000 years, and (d) 1,000,000 years.

SUMMARY AND CONCLUSIONS

Development of an enhanced performance assessment (PA) capability for geologic disposal of SNF and HLW has been ongoing for several years in the U.S. repository program. The new Generic Disposal System Analysis (GDSA) modeling and software framework is intended to be flexible enough to evolve through the various phases of repository activities, beginning with generic PA activities in the current Concept Evaluation phase to site-specific PA modeling in the Repository Development phase. The GDSA Framework utilizes modern software and hardware capabilities by being based on open-source software architecture and being configured to run in a massively parallel, high-performance computing (HPC) environment. It consists of two main components, the open-source Dakota uncertainty sampling and analysis software and the PFLOTRAN reactive multi-phase flow and transport simulator.

Reference cases or "generic repositories" have been, and are being developed, based on typical properties for potential salt, clay, and granite host-rock formations and corresponding engineered design concepts for each medium. Past simulations have focused on a generic repository in bedded-salt host rock, while the most recent research has focused on a reference case for a typical clay/shale host rock. A variety of single-realization (i.e., deterministic) and multi-realization (probabilistic) results for the new clay reference case are presented, including an analysis of the effects of heat generation on repository performance, assuming a 100-year out-of-reactor

commercial SNF waste form. Order-of-magnitude differences between predicted radionuclide concentrations in thermal versus isothermal simulations imply that mechanistic, coupled-process modeling in three-dimensional (3-D) domains can be important for building confidence in post-closure performance assessments. Although the proof-of-principle simulations provide preliminary insights into the effect of multi-physics processes and thermal-hydrologic coupling on the long-term behavior of a reference-case clay repository, additional refinements are necessary before they are used as a definitive guide for future R&D.

Progress in the development of the GDSA Framework continues to affirm that HPC-capable codes can be used to simulate important multi-physics couplings directly in a total system performance assessment of a deep geologic repository. The generic repository applications modeled to date indicate that the developing capability can simulate complex coupled processes in a multi-kilometer domain while simultaneously simulating the coupled behavior of meter-scale features, including every waste package within the domain.

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