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

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ABSTRACT

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. 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. This evolution demands that total system performance assessment (PA) models be flexible enough to accommodate the associated advances, which is the motivation behind 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. At present, DOE's enhanced PA capability is being applied to a variety of generic disposal concepts, including mined disposal in salt, clay/shale, and granite formations, and deep borehole disposal in granite formations. 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:

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

Regarding Function #1, increased confidence and transparency in the repository safety case will be fostered by two important features of the new enhanced PA model: (1) less reliance on assumptions and simplifications ("abstractions"), i.e., more direct representation of multi-physics couplings in a performance assessment; and (2) realistic spatial resolution of features and processes, including direct representation of all emplaced waste packages. Advances in hardware and software facilitate both of these goals, i.e., the goals of greater process resolution and greater spatial-temporal resolution, and are being reflected in the new PA model.

The new PA modeling framework incorporates two main software components that are optimized for parallel computations in an HPC environment: DAKOTA for uncertainty quantification and propagation and PFLOTRAN for multi-physics domain simulation. Deterministic simulations (single-realization) are run using "best estimate" generic parameter values for waste degradation and groundwater flow and radionuclide transport under undisturbed repository conditions (e.g., no human intrusions). For probabilistic simulations, parameter (and potentially model) uncertainty are taken into account using probability distributions that are propagated through the system via a Monte Carlo approach in DAKOTA. Classical sensitivity analysis (e.g., rank regression) has been utilized to identify the most important parameters. It is intended that insights gained from future such sensitivity analyses will be used to guide and prioritize ongoing R&D, which is Function #2 above.

Regarding Function #3, evaluation of potential disposal concepts, the work reported here presents applications of the GDSA Framework to two of the generic concepts: disposal in bedded salt and disposal in an argillaceous medium. Previously reported work has described simulations for a bedded salt reference case using a three-dimensional (3-D) grid domain that was effectively "quasi 2-D" because it was applied to only the central disposal drift. The current work expands on this by simulating multiple disposal drifts in 3-D in a generic bedded salt repository, including both deterministic and probabilistic cases, where the latter propagates uncertainties in about ten key input parameters to uncertainty in radionuclide concentration in a representative aquifer. Comparisons of repository performance are made between a multi-drift, 3-D case with heat-generating waste ("thermal" case) and a multi-drift, 3-D case without heat generation ("isothermal" case), using commercial SNF as the source term in a bedded salt host rock. The enhanced PA modeling framework is also applied to a newly developed "clay/argillite" reference case, which illustrates the performance of a host rock with much lower thermal conductivity than bedded salt. In addition, the PA model is tested by application to a bedded-salt repository that contains only DOE-managed HLW.

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