SAND2013-6183P

Performance Assessment Modeling of a Generic Salt Disposal System: Annotated Outline

Fuel Cycle Research & Development

Prepared for
U.S. Department of Energy
Used Fuel Disposition

G. Freeze, P. Gardner, P. Vaughn, S.D. Sevougian, P. Mariner, V. Mousseau
Sandia National Laboratories

July 2013
FCRD-UFD-2013-000219
SAND2013-xxxxP

Sandia National Laboratories

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

FCT Quality Assurance Program Document

Appendix E
FCT Document Cover Sheet

Name/Title of Deliverable/Milestone	Performance Assessment Modeling of a Generic Salt Disposal System: Annotated Outline, M4FT-13SN0808045
Work Package Title and Number	Generic Disposal System Level Modeling, FT-13SN080804
Work Package WBS Number	1.02.08.08
Responsible Work Package Manager	Geoff Freeze (Name/Signature)

Date Submitted November 16, 2012

Quality Rigor Level for Deliverable/Milestone	☐ QRL-3	☐ QRL-2	☐ QRL-1 ☐ Nuclear Data	☒ N/A*

This deliverable was prepared in accordance with Sandia National Laboratories *(Participant/National Laboratory Name)*

QA program which meets the requirements of

☒ DOE Order 414.1 ☐ NQA-1-2000

This Deliverable was subjected to:

☒ Technical Review

☐ Peer Review

Technical Review (TR)

Review Documentation Provided

☐ Signed TR Report or,

☐ Signed TR Concurrence Sheet or,

☒ Signature of TR Reviewer(s) below

Peer Review (PR)

Review Documentation Provided

☐ Signed PR Report or,

☐ Signed PR Concurrence Sheet or,

☐ Signature of PR Reviewer(s) below

Name and Signature of Reviewers

*Note: In some cases there may be a milestone where an item is being fabricated, maintenance is being performed on a facility, or a document is being issued through a formal document control process where it specifically calls out a formal review of the document. In these cases, documentation (e.g., inspection report, maintenance request, work planning package documentation or the documented review of the issued document through the document control process) of the completion of the activity along with the Document Cover Sheet is sufficient to demonstrate achieving the milestone. QRL for such milestones may be also be marked N/A in the work package provided the work package clearly specifies the requirement to use the Document Cover Sheet and provide supporting documentation.

CONTENTS

FIGURES

ACRONYMS

ADSM	advanced disposal system modeling
DOE	U.S. Department of Energy
DRZ	disturbed rock zone
EBS	engineered barrier system
FEP	feature, event, and process
FY	fiscal year
GDSM	generic disposal system modeling
HLW	high-level radioactive waste
HPC	high-performance computing
NBS	natural barrier system
NE	Office of Nuclear Energy
NRC	U.S. Nuclear Regulatory Commission
QA	quality assurance
THC	thermal-hydrologic-chemical
THCMBR	thermal-hydrologic-chemical-mechanical-biological-radiological
PA	performance assessment
R&D	research and development
UFDC	Used Fuel Disposition Campaign
UNF	used nuclear fuel
V&V	verification and validation

1. INTRODUCTION

The Used Fuel Disposition Campaign (UFDC) of the U.S. Department of Energy (DOE) Office of Nuclear Energy (NE) is conducting research and development (R&D) on generic deep geologic disposal systems (i.e., repositories) for high-activity nuclear wastes that exist today or that could be generated under future fuel cycles. The term high-activity waste (U.S. Nuclear Waste Technical Review Board 2011) refers collectively to both used nuclear fuel (UNF) from nuclear reactors and high-level radioactive waste (HLW) from reprocessing of UNF, and from other sources.

Generic Disposal System Modeling (GDSM) and Advanced Disposal System Modeling (ADSM) Work Package activities completed in Fiscal Year (FY) 2012 and prior years demonstrated the capability to perform generic disposal system simulations for salt, clay/shale, granite, and deep borehole disposal options. These capabilities are documented in Clayton et al. (2011), Freeze and Vaughn (2012), and Vaughn et al. (2013).

This report provides an annotated outline of specific activities performed in FY2013 contributing to the development of an advanced disposal system modeling capability and its application, for demonstration purposes, to a generic salt disposal system. The report addresses the following GDSM Work Package milestone:

- *Level 4 Milestone* – Generic Modeling of Deep Borehole and Salt (M4FT-13SN0808045)

Full text to address the annotated outline of this report will be part of the following GDSM Work Package milestone, to be completed in November 2013:

- *Level 2 Milestone* – Generic Disposal System Modeling Report (M2FT-13SN0808043)

The annotated outline for the generic salt disposal system model is presented in Section 2. A summary and conclusions is presented in Section 3.

The Level 4 Milestone noted above was planned to also include generic deep borehole disposal system modeling. However, that work will be documented in a separate Level 2 Milestone as part of the UFDC Deep Borehole Disposal Disposal R&D Work Package.

2. GENERIC SALT DISPOSAL SYSTEM MODEL

In FY2012, a simplified salt disposal system model was developed (Vaughn et al. 2013, Sections 3.1 and 3.5), the requirements for an advanced performance assessment (PA) modeling capability were identified (Freeze and Vaughn 2012; Vaughn et al. 2013, Section 2), and an initial design and requirements for an advanced PA model to support safety assessments for the disposal of high-activity waste in a mined geologic repository at a generic salt site were described (Sevougian et al. 2012).

The continuing development of the advanced salt repository PA model is documented in this report. The documentation is in the form of an annotated outline. The annotated outline identifies the technical content which will be fully developed in a subsequent Level 2 Milestone, deliverable in November 2013.

Section 2.1 describes the PA model framework, Section 2.2 describes a generic salt repository reference case used for an initial demonstration of PA model capability, and Section 2.3 presents preliminary model results.

The following definitions are provided to ensure consistent understanding of terminology used throughout the report:

- **Conceptual model—**A representation of the behavior of a real-world process, phenomenon, or object as an aggregation of scientific concepts, so as to enable predictions about its behavior. Such a model consists of concepts related to geometrical elements of the object (size and shape); dimensionality (one-, two-, or three-dimensional (1D, 2D, or 3D)); time dependence (steady-state or transient); applicable conservation principles (mass, momentum, energy); applicable constitutive relations; significant processes; boundary conditions; and initial conditions (NRC 1999, Appendix C).
- **Mathematical model—**A representation of a conceptual model of a system, subsystem, or component through the use of mathematics. Mathematical models can be mechanistic, in which the causal relations are based on physical conservation principles and constitutive equations. In empirical models, causal relations are based entirely on observations (NRC 1999, Appendix C).
- **Numerical model—**An approximate representation of a mathematical model that is constructed using a numerical description method such as finite volumes, finite differences, or finite elements. A numerical model is typically represented by a series of program statements that are executed on a computer (NRC 2003, Glossary).
- **Computer code—**An implementation of a mathematical model on a digital computer generally in a higher-order computer language … (NRC 1999, Appendix C).
- **Performance assessment (PA) model—**A PA model derives from the steps of a PA methodology (Meacham et al. 2011, Section 1): feature, event, and process (FEP) analysis; scenario construction; uncertainty quantification; and development of an integrated system model (incorporating conceptual, mathematical, and numerical model considerations). The PA model includes the mathematical and numerical implementation of the conceptual description of the disposal system components and their interactions. To perform calculations with a PA model, a computer code that implements the numerical model must be utilized.

2.1 PA Model Framework

This section will describe the advanced PA model framework supporting generic salt disposal system modeling, including the application to a salt repository demonstration problem. The two main components of a PA model framework are (Freeze and Vaughn 2012, Section 2):

- A *conceptual multi-physics model framework* that facilitates development of
  - a conceptual model of the important FEPs and scenarios that describe the multi-physics phenomena of a specific disposal system (e.g., a salt repository) and its subsystem components, and
  - a mathematical model (e.g., governing equations) that implements the representations of the important FEPs and their couplings.
- A *computational framework* that facilitates integration of
  - the system analysis workflow (e.g., input pre-processing, integration and numerical solution of the mathematical representations of the conceptual model components, output post-processing), and
  - the supporting capabilities (e.g., mesh generation, input parameter specification and traceability, matrix solvers, visualization, uncertainty quantification and sensitivity analysis, file configuration management including verification and validation (V&V) and quality assurance (QA) functions, and compatibility with high-performance computing (HPC) environments).

The conceptual multi-physics model framework supports conceptual model development and integration of the various submodels of each of the disposal system components. Development of the conceptual model framework is described in Section 2.1.1. The computational framework supports the numerical model and computer code implementation, including advanced modeling and HPC considerations. Development of the computational framework is described in Section 2.1.2.

2.1.1 Conceptual Model Framework

This section will describe the development of the salt repository conceptual model for the demonstration problem. Components of the conceptual model that will be described include:

- Specification of the regions and features of the generic salt disposal system (Section 2.1.1.1)
- Identification and preliminary screening of potentially relevant FEPs (Section 2.1.1.2)
- Development of scenarios (undisturbed and disturbed) (Section 2.1.1.3)

2.1.1.1 Generic Salt Repository Regions and Features

The regions and features of the generic salt disposal system will be updated from Sevougian et al. (2012, Section 3.1.1).

The regions of a generic salt repository, shown in Figure 2-1, include: the Engineered Barrier System (EBS); the Natural Barrier System (NBS) or Geosphere; and the Biosphere. Figure 2-1 schematically illustrates the nested 3D nature of the disposal system. The NBS completely surrounds the EBS (which encompasses the waste and emplacement tunnels, shown in red in the figure); radionuclides can be transported from the waste through the EBS and the NBS to the biosphere along multiple flow pathways.

The features of each of the regions of a generic salt repository are shown schematically in 1D in

Figure 2-2. The features of the EBS include the wastes (e.g., inventory and waste forms) and engineered features (e.g., waste package, crushed salt backfill, and seals); the features of the NBS include the disturbed rock zone (DRZ), host rock (e.g., halite with anhydrite interbeds and clay seams), and other geological units (e.g., overlying or underlying aquifers); and the features of the biosphere include the surface environment and receptor characteristics. 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. Immediately adjacent to the EBS, these repository-induced changes are more likely to be permanent (e.g., mechanical alteration due to excavation), whereas further from the EBS the repository-induced changes are more likely to be time-dependent but not permanent (e.g., thermal effects due to radioactive decay of waste). The DRZ is sometimes referred to as the excavation disturbed zone (EDZ). However, in this report, DRZ is preferred because it more accurately represents the fact that the disturbed zone includes effects from both excavation and waste emplacement. Alternate terms that are commonly used to describe a disposal system, "near field" and "far field", are also shown in

Figure 2-2. The near field encompasses the EBS and the DRZ (i.e., the components influenced by the presence of the repository). The far field encompasses the remainder of the NBS (i.e., beyond the influence of the repository).

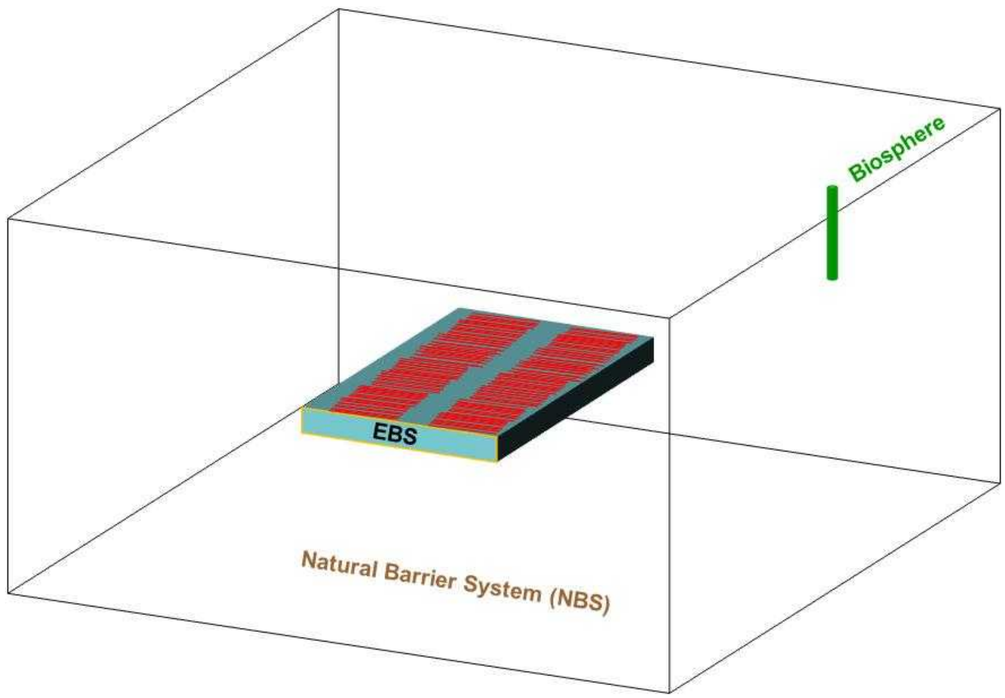

Figure 2-1. Regions of Generic Salt Disposal System

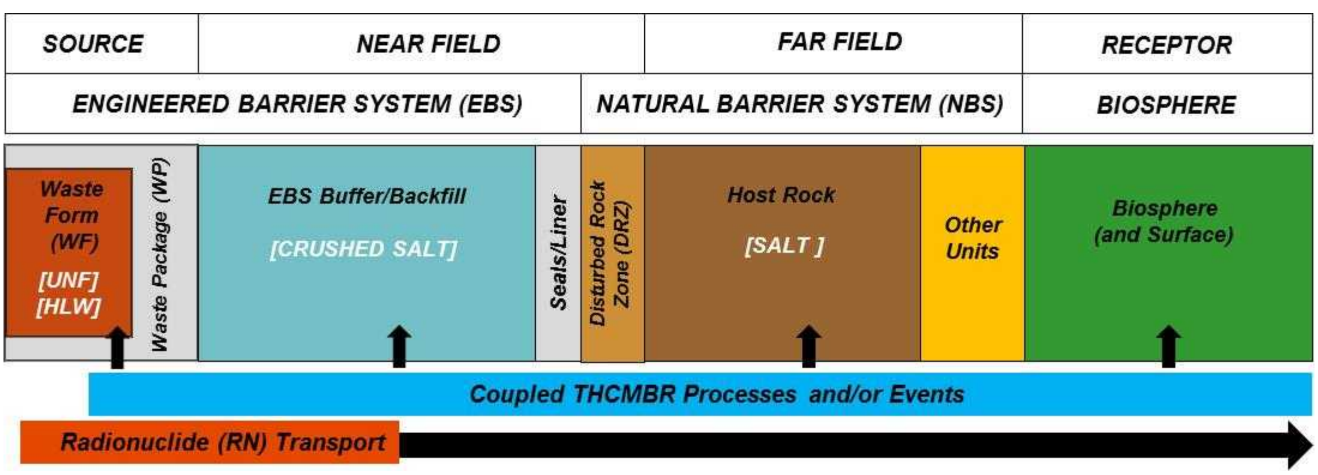

Figure 2-2. Features and Phenomena of a Generic Salt Disposal System

Figure 2-2 also illustrates schematically how radionuclide movement from the waste form to the receptor is influenced by multi-physics phenomena that can act upon and within each of the regions and/or features. These multi-physics phenomena include, at a high level, the thermal-hydrologic-chemical-mechanical-biological-radiological (THCMBR) processes and external events (e.g., seismicity) that describe (1) waste form and waste package degradation, (2) radionuclide mobilization from the waste form and radionuclide release from the waste package (identified as the radionuclide source in Figure 2-2), (3) radionuclide transport through the near field and far field, and (4) radionuclide transport, uptake, and health effects in the biosphere. In addition to their direct effects on radionuclide transport, the THCMBR processes also influence the physical and chemical environments (e.g., temperature, fluid chemistry, biology, mechanical alteration) in the EBS, NBS, and biosphere, which in turn affect water movement, degradation of EBS components, and radionuclide transport.

2.1.1.2 Generic Salt Repository FEP Analysis

The identification and preliminary screening of potentially relevant FEPs will be updated from Sevougian et al. (2012, Section 3.1.2 and Appendix A) and from Freeze et al. (2013).

A list of 208 FEPs potentially relevant to a generic salt repository was compiled by Sevougian et al. (2012, Appendix A), based on a generic UFDC FEP list (Freeze et al. 2011, Appendix A). Sevougian et al. (2012, Appendix A) identified preliminary screening recommendations for these FEPs (e.g., included, excluded, site- and/or design-specific information needed, or further technical evaluation needed), based on a generic salt repository reference design (see Section 2.2). Figure 2-3 provides a schematic illustration of the key phenomena (representative of the likely included FEPs) identified as important to the long-term performance of a generic salt repository under undisturbed conditions. Further discussion of disturbed scenarios is provided in Section 2.1.1.3.

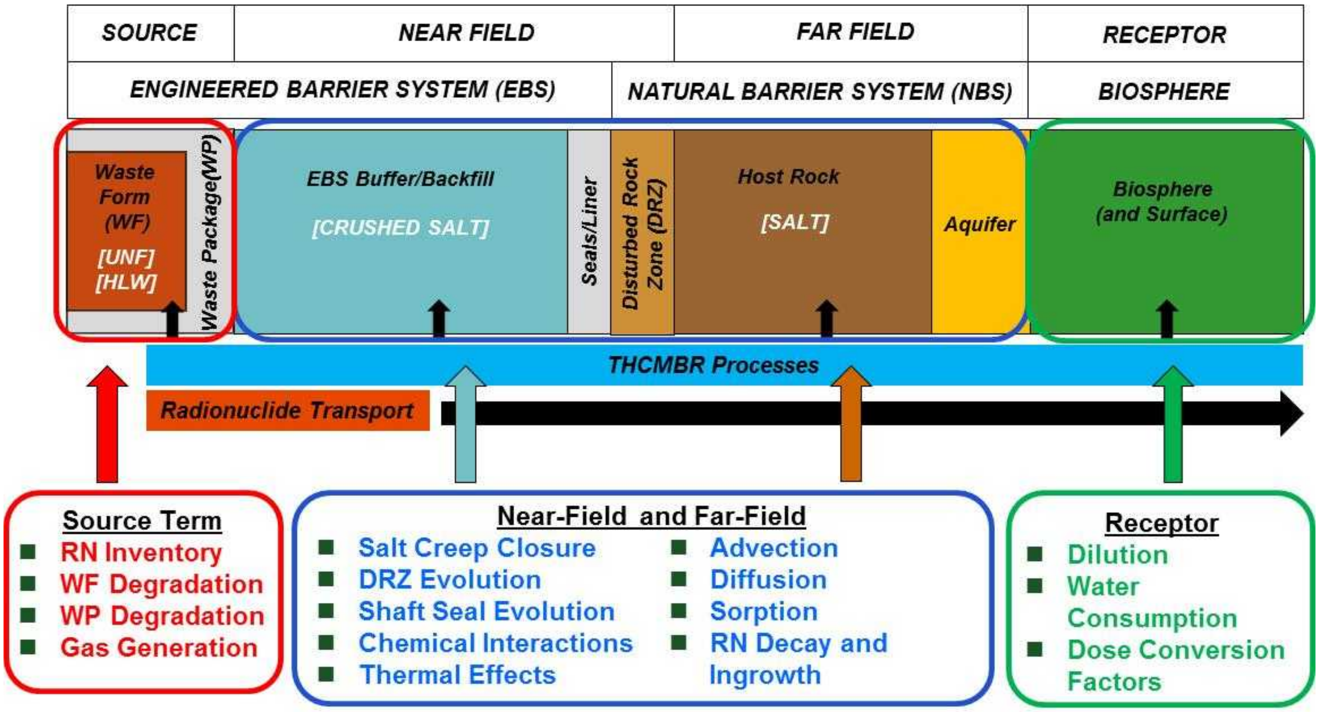

Figure 2-3. Key Phenomena in a Generic Salt Repository (Undisturbed Scenario)

Freeze et al. (2013) presented a new FEP classification methodology, using a 2D matrix structure, to organize the 208 generic salt repository FEPs. The application of the FEP matrix approach could result in changes to the scope of some of the salt repository FEPs. Results of updated FEP scope and screening will be documented in the GDSM Level 2 Milestone in November 2013.

2.1.1.3 Generic Salt Repository Scenario Development

The development of undisturbed and disturbed scenarios will be updated from Sevougian et al. (2012, Section 3.1.3).

The current focus is on undisturbed scenarios.

2.1.2 Computational Framework

This section will describe the development of the computational framework supporting the salt repository model demonstration problem. Components of the computational framework that will be described include:

- System analysis workflow and computational capabilities (Section 2.1.2.1)
- Configuration management (Section 2.1.2.2)

Details of the annotated outline for the computational framework will be provided in the following ADSM Work Package milestone:

- *Level 3 Milestone* – Advanced Modeling Report (M3FT-13SN0808062)

An abbreviated outline is provided here.

2.1.2.1 System Analysis Workflow and Computational Capabilities

As outlined in Freeze and Vaughn (2012, Section 2.3), the system analysis workflow and computational capabilities control the development and execution of the integrated system PA model. Specific functions include:

- Input development and pre-processing (spatial and temporal discretization, mesh generation, input parameter specification and traceability including uncertainty)
- System model development and implementation (mathematical representations of process model FEPs and couplings, uncertainty quantification)
- Integrated system model execution (numerical representations of FEPs and couplings, data structure and matrix solvers)
- Output management and post-processing (analysis of results, visualization, sensitivity analyses)

This section will describe the implementation of the following open-source codes to perform these functions in support of the generic salt repository PA model:

- DAKOTA – sensitivity analysis and uncertainty quantification
- LIME – numerical coupling of multi-physics codes
- PFLOTRAN – THC multi-physics flow and transport

The relationship between these codes is shown in Figure 2-4. In addition to the codes listed above, the following capabilities are also required:

- Source Term Definition – An "EBS Evolution" code to represent the inventory, waste form, and waste package degradation multi-physics processes contributing to the radionuclide source term
- Biosphere Transport and Receptor Uptake – A "Biosphere Receptor" code to represent the surface and biosphere processes contributing to the dose to a human receptor resulting from radionuclide releases from the NBS.
- Mesh Generation – Cubit or similar code
- Visualization – VisIT or similar code
- Scripting – Python scripts to process output data for analysis

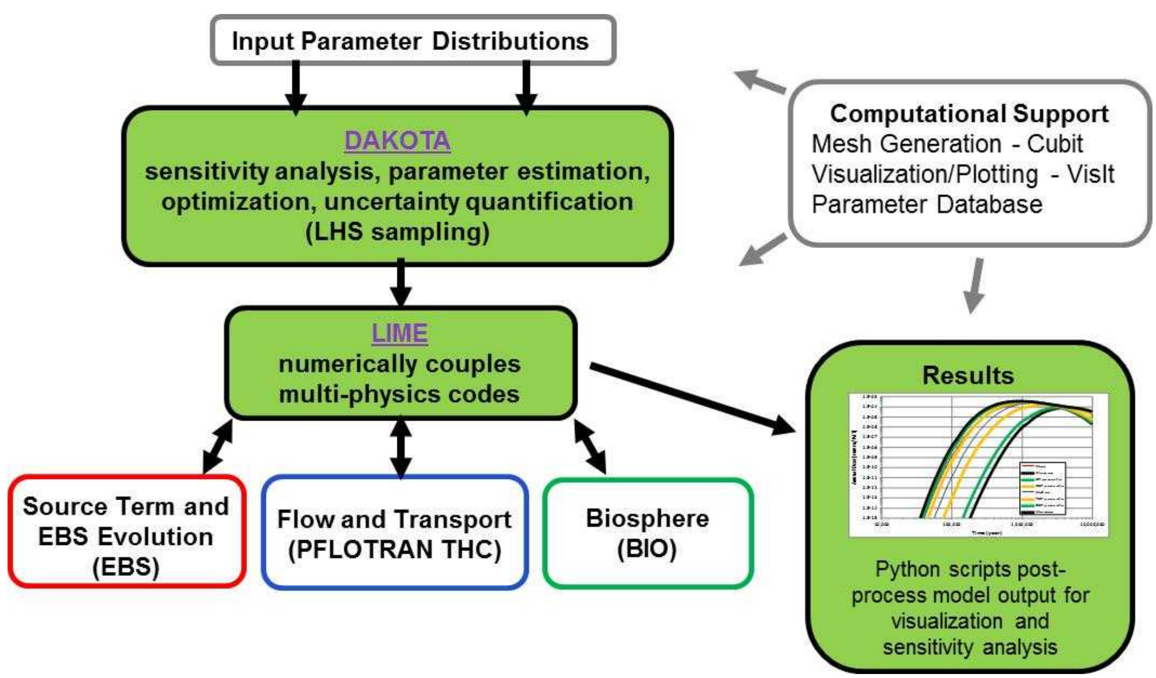

Figure 2-4. PA Model Framework Integrated Codes

2.1.2.2 Configuration Management

As outlined in Freeze and Vaughn (2012, Section 2.3), the configuration management component of the computational framework supports the following:

- Input development (parameter database, file access and storage)
- Output management (file access and storage)

This section will describe the configuration management tools and practices supporting the salt repository demonstration problem.

2.2 Generic Salt Repository Reference Case

As described in Sevougian et al. (2012, Section 3.2), the generic salt repository reference case has the following major elements:

- Waste inventory
- Geologic disposal system: Engineered Barrier System
- Geologic disposal system: Natural Barrier System
- Concept of operations
- Biosphere
- Regulatory environment

These major elements of the salt repository reference case will be updated from Sevougian et al. (2012, Section 3.2).

2.2.1 Waste Inventory

This section will describe the radionuclide inventory from UNF and/or HLW used in the salt repository demonstration problem reference case. It will be updated from Sevougian et al. (2012, Sections 3.2.1 and 3.2.2.1) and from Carter et al. (2012).

2.2.2 Concept of Operations

This section will describe the concept of operations that define the salt repository demonstration problem reference case. It will be updated from Sevougian et al. (2012, Section 3.2.4).

The description of the concept of operations will include:

- Waste package type and emplacement mode
- Repository layout and tunnel/drift design

- Thermal constraints

2.2.3 Geologic Disposal System: Engineered Barrier System

This section will describe the EBS used in the salt repository demonstration problem reference case. It will be updated from Sevougian et al. (2012, Section 3.2.2).

The description of the EBS will include the following components:

- Waste form
- Waste package
- Backfill
- Seals

2.2.4 Geologic Disposal System: Natural Barrier System

This section will describe the bedded salt NBS used in the salt repository demonstration problem reference case. It will be updated from Sevougian et al. (2012, Section 3.2.3).

The description of the NBS will include the geometry and THC characteristics of the following components:

- Disturbed rock zone
- Host rock (repository horizon relatively pure halite)
- Host rock interbeds (anhydrite layers and/or clay seams)
- Aquifer
- Regions of over-pressurization

2.2.5 Biosphere

This section will describe the biosphere used in the salt repository demonstration problem reference case. It will be updated from Sevougian et al. (2012, Section 3.2.5).

The description of the biosphere will include:

- Biosphere characteristics
- Receptor characteristics

2.2.6 Regulatory Environment

This section will describe the regulatory assumptions for salt repository demonstration problem reference case. It will be updated from Sevougian et al. (2012, Section 3.2.6).

The regulatory assumptions will address:

- FEP screening criteria
- Retrievability
- Biosphere and receptor characteristics
- Radionuclide release and/or dose limits
- Human intrusion

2.3 Application of the Salt Disposal System Model

This section will describe simulation results from the application of the advanced PA model framework described in Section 2.1 to the salt repository reference case described in Section 2.2.

The model domain for the demonstration problem, shown in Figure 2-5, includes an EBS – consisting of waste, disposal tunnels/drifts (shown in red), and a shaft, and a NBS – consisting of a DRZ, host rock halite, anhydrite interbeds (one above the EBS and one below the EBS), and an overlying aquifer. The biosphere (accessible environment) is assumed to be located at the ground surface. The receptor is assumed to be located at the ground surface, at a distance of 5,000 m laterally from the disposal area.

The reference salt repository is assumed to contain approximately 70,000 metric tons heavy metal (MTHM), distributed throughout 76 pairs of disposal tunnels/drifts, where each of the 152 tunnels is 800 m long and contains 80 waste packages of UNF. Figure 2-6 shows the waste package configuration within a single tunnel.

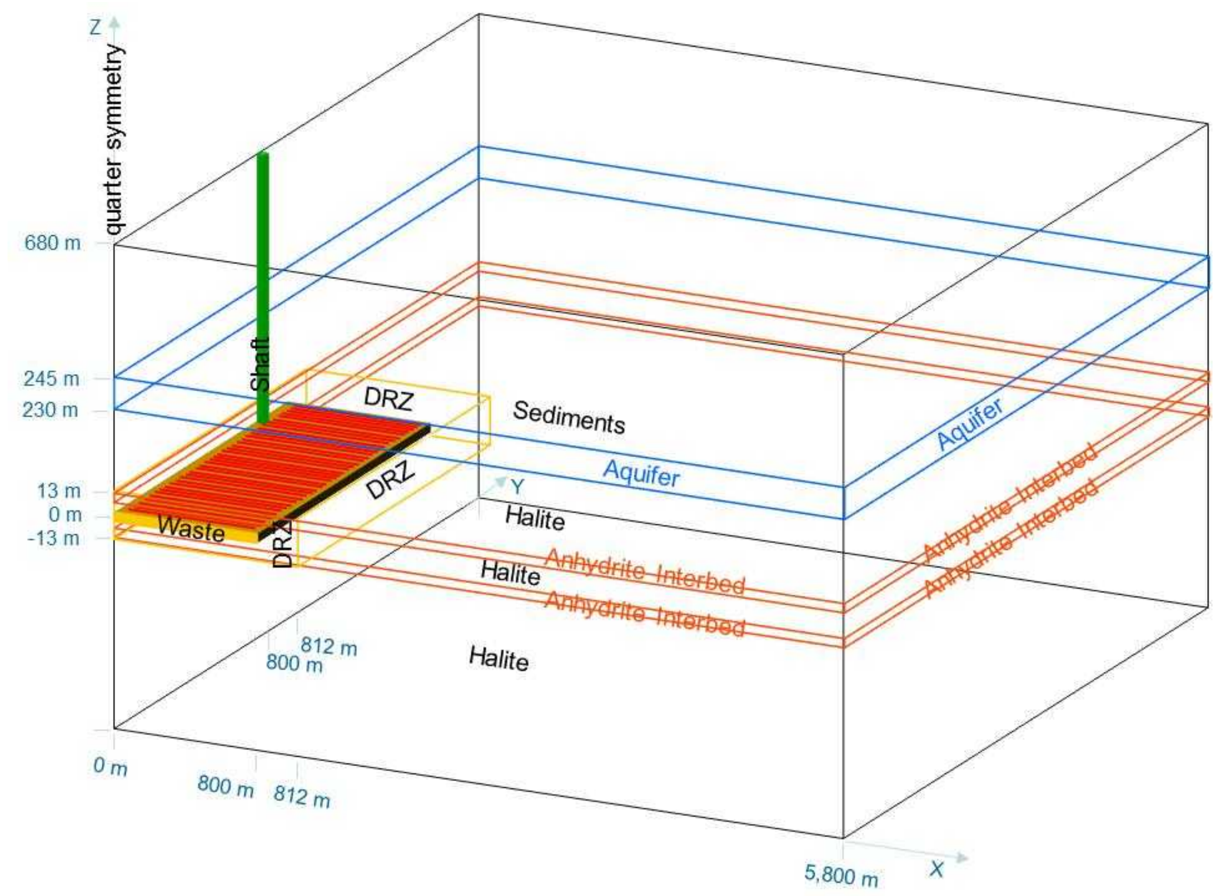

Figure 2-5. Salt Repository Demonstration Problem Model Domain

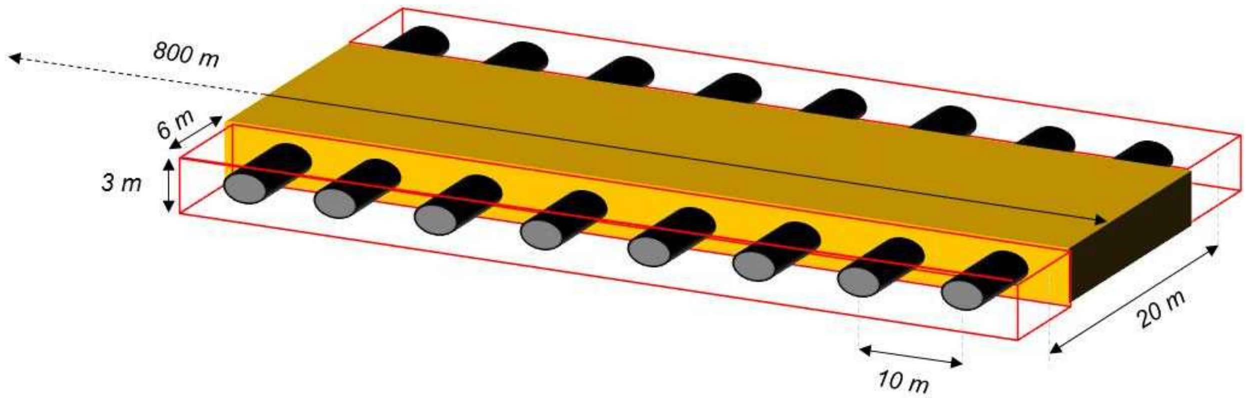

Figure 2-6. Salt Repository Demonstration Problem Tunnel Configuration

The model domain in Figure 2-5 takes advantage of one-quarter horizontal symmetry; it shows 38 disposal tunnels (one-quarter of the total). However, for the demonstration problem model, only the outer 100 m of a single drift was simulated. Within the single drift, waste form degradation is fast (half of the waste from is degraded in 100 years) and waste package degradation is assumed to be instantaneous. The properties of the reference case result in two primary radionuclide transport pathways to the biosphere:

- Diffusion out the DRZ and subsequent advection through the interbeds
- Diffusion up the shaft and subsequent advection through the aquifer

Transport in the host rock halite is by diffusion. Transport includes the effects of sorption and decay and ingrowth. ^{129}I is the dominant radionuclide because it has unlimited solubility and is non-sorbing.

The undisturbed scenario results include a deterministic baseline simulation (Section 2.3.1) and probabilistic sensitivity simulations (Section 2.3.2). The demonstration problem simulations were performed on the Sandia National Laboratories (SNL) Red Sky HPC cluster.

2.3.1 Deterministic Baseline Simulation Results

This section will describe the deterministic baseline simulation results from the salt repository demonstration problem.

The deterministic simulation used specified values for all parameters; for uncertain parameters mean values were typically used. Results are shown in form of ^{129}I dissolved concentration as a function of time and space. An example is shown in Figure 2-7.

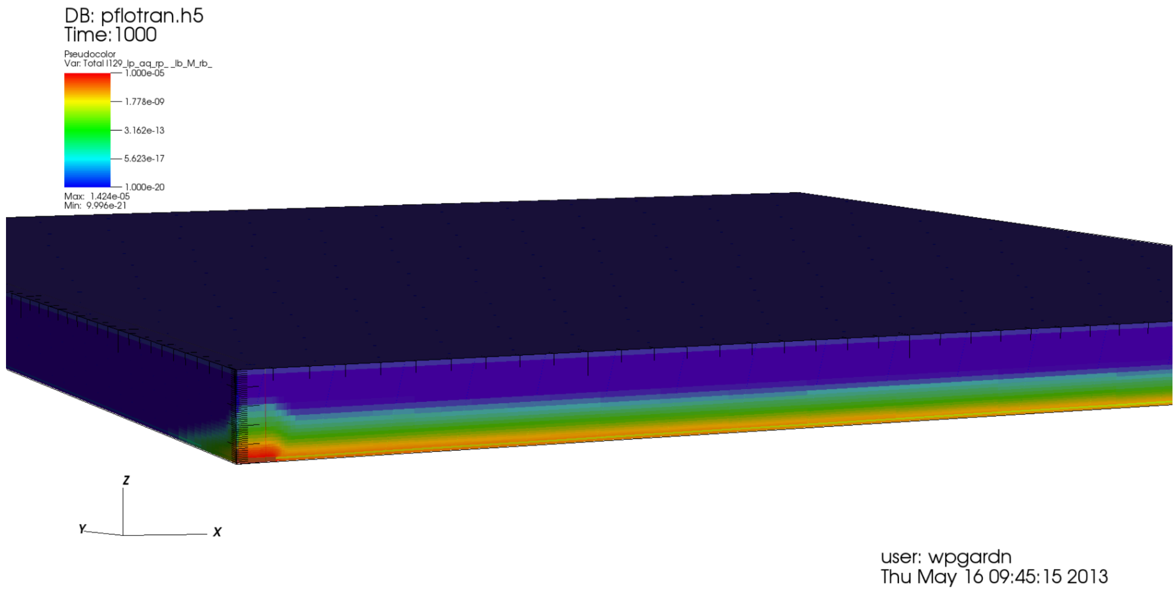

Figure 2-7. Example of ^{129}I Dissolved Concentration at a Specified Time for the Salt Repository Reference Case

2.3.2 Probabilistic Sensitivity Simulation Results

This section will describe the probabilistic sensitivity simulation results from the salt repository demonstration problem.

The sensitivity simulations use sampled values for a selected set of uncertain parameters. Parameter sampling and sensitivity analyses are performed using DAKOTA. Results may shown in form of horsetail plots of ^{129}I dissolved concentration, rank correlations, and scatter plots.

3. SUMMARY AND CONCLUSIONS

This section will summarize the development and application of the salt repository PA model and discuss conclusions and future work to enhance the advanced PA modeling capabilities.

4. REFERENCES

Carter, J. T., A. J. Luptak, J. Gastelum, C. Stockman, and A. Miller 2012. *Fuel Cycle Potential Waste Inventory for Disposition*. FCRD-USED-2010-000031, Rev. 5.

Clayton, D., G. Freeze, T. Hadgu, E. Hardin, J. Lee, J. Prouty, R. Rogers, W.M. Nutt, J. Birkholzer, H.H. Liu, L. Zheng, and S. Chu 2011. *Generic Disposal System Modeling – Fiscal Year 2011 Progress Report.* FCRD-USED-2011-000184, SAND2011-5828P. U.S. Department of Energy, Office of Nuclear Energy, Used Fuel Disposition Campaign, Washington, D.C.

Freeze, G. and P. Vaughn 2012. *Development of an Advanced Performance Assessment Modeling Capability for Geologic Disposal of Nuclear Waste: Methodology and Requirements.* SAND2012-10208. Sandia National Laboratories, Albuquerque, New Mexico.

Freeze, G., S.D. Sevougian, and M. Gross 2013. *Safety Framework for Disposal of Heat-Generating Waste in Salt: Features, Events, and Processes (FEPs) Classififcation.* FCRD-UFD-2013-000191. SAND2013-5220P. Sandia National Laboratories, Albuquerque, New Mexico.

Sevougian, S.D., G.A. Freeze, M.B. Gross, J. Lee, C.D. Leigh, P. Mariner, R.J. MacKinnon, and P. Vaughn 2012. *TSPA Model Development and Sensitivity Analysis of Processes Affecting Performance of a Salt Repository for Disposal of Heat-Generating Nuclear Waste*. FCRD-UFD-2012-000320 Rev. 0, U.S. Department of Energy, Office of Nuclear Energy, Used Nuclear Fuel Disposition, Washington, D.C.

U.S. Nuclear Regulatory Commission (NRC) 1999. *Regulatory Perspectives on Model Validation in High-Level Radioactive Waste Management Programs: A Joint NRC/SKI White Paper*. NUREG-1636. U.S. Nuclear Regulatory Commission, Washington, DC.

U.S. Nuclear Regulatory Commission (NRC) 2003. *Yucca Mountain Review Plan*. NUREG-1804, Revision 2. Office of Nuclear Material and Safeguards, Washington, DC.

U.S. Nuclear Waste Technical Review Board. 2011. *Technical Advancements and Issues Associated with the Permanent Disposal of High Activity Wastes, Lessons Learned from Yucca Mountain and Other Programs*. June.

Vaughn, P., G. Freeze, J. Lee, S. Chu, K.D. Huff, W.M. Nutt, T. Hadgu, R. Rogers, J. Prouty, E. Hardin, B. Arnold, E. Kalinina, W.P. Gardner, M. Bianchi, H.H. Liu, and J. Birkholzer 2013. *Generic Disposal System Model: Architecture, Implementation, and Demonstration.* FCRD-UFD-2012-000430 Rev. 1, SAND2013-1539P. Sandia National Laboratories, Albuquerque, New Mexico.