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Evaluation of Advanced Performance Assessment Modeling Frameworks: Annotated Outline

Fuel Cycle Research & Development

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

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Appendix E
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☒ DOE Order 414.1 ☐ NQA-1-2000

This Deliverable was subjected to:

☒ Technical Review	☐ Peer Review
Technical Review (TR)	**Peer Review (PR)**
Review Documentation Provided	**Review Documentation Provided**
☐ Signed TR Report or,	☐ Signed PR Report or,
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ACRONYMS

ADSM	advanced disposal system modeling
DAKOTA	Design Analysis toolKit for Optimization and Terascale Applications
DOE	U.S. Department of Energy
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
LIME	Lightweight Integrating Multi-Physics Environment
NBS	natural barrier system
NE	Office of Nuclear Energy
NRC	U.S. Nuclear Regulatory Commission
QA	quality assurance
THC	thermal-hydrologic-chemical
PA	performance assessment
PETSc	Portable Extensible Toolkit for Scientific Computation
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. The report addresses the following ADSM Work Package milestone:

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

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 advanced disposal system modeling capability is presented in Section 2. A summary and conclusions is presented in Section 3.

2. GENERIC SALT DISPOSAL SYSTEM MODEL

In FY2012, 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 repository PA modeling capabilities 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.

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 disposal system modeling. 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 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 a generic repository conceptual model for a demonstration problem. The regions of a generic repository are shown in Figure 2-1. They 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.

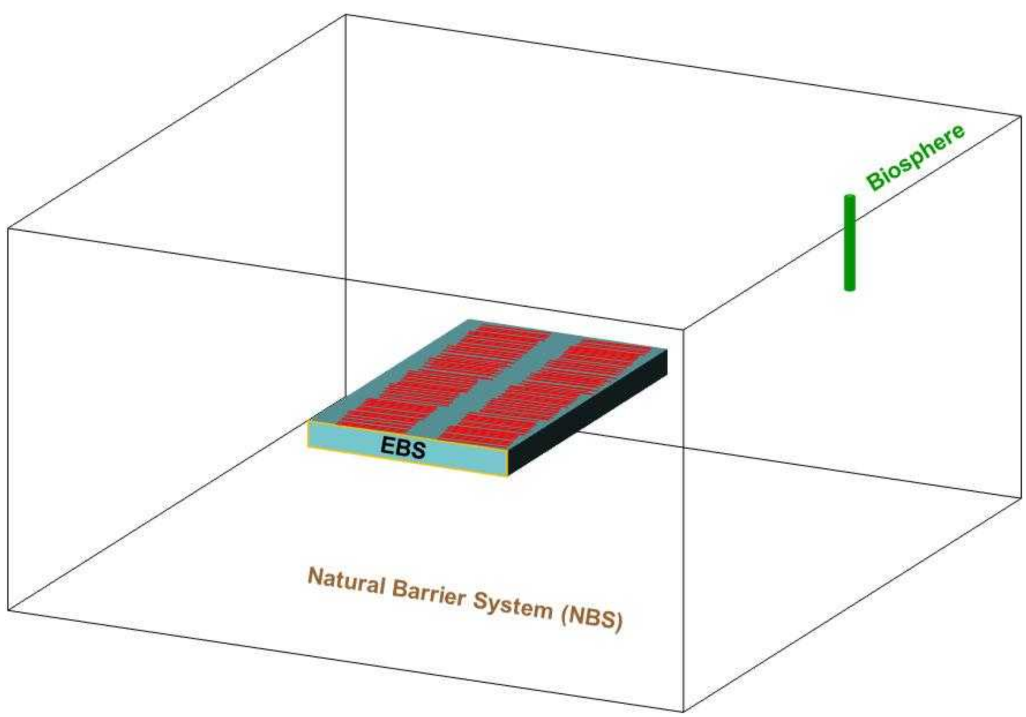

Figure 2-1. Regions of Generic Disposal System

Components of the conceptual model that will be described in this section 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)

Details of the annotated outline for this conceptual model framework section and subsections are provided in the following GDSM Work Package milestone (Freeze et al. 2013) and are not reproduced here:

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

2.1.2 Computational Framework

This section will describe the development of the computational framework supporting geenric 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)

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 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 2-2. 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

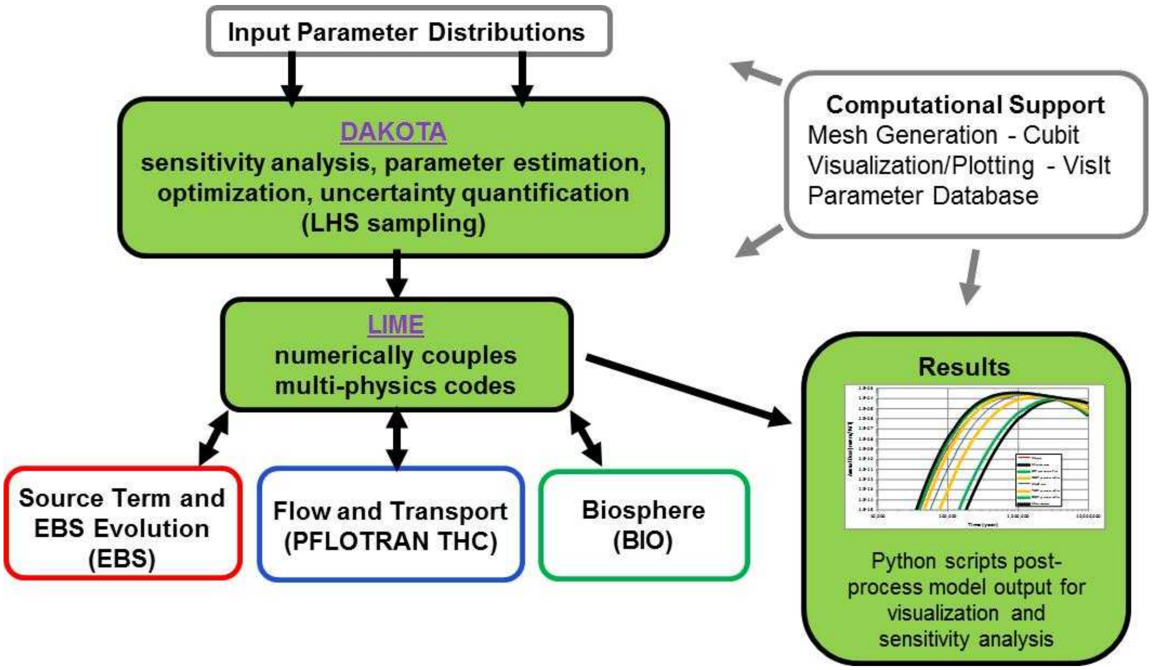

Figure 2-2. PA Model Framework Integrated Codes

Details of these codes are provided in subsequent subsections.

2.1.2.1.1 DAKOTA

This section will describe the DAKOTA capabilities used to support an advanced PA model framework.

DAKOTA (Design Analysis toolKit for Optimization and Terascale Applications) (Adams et al. 2013a; Adams et al. 2013b) manages uncertainty quantification, sensitivity analyses, optimization, and calibration. Specific capabilities include (

Figure 2-3):

- Generic interface to simulations
- Extensive library of time-tested and advanced algorithms
- Mixed deterministic / probabilistic analysis
- Supports scalable parallel computations on clusters
- Object-oriented code; modern software quality practices

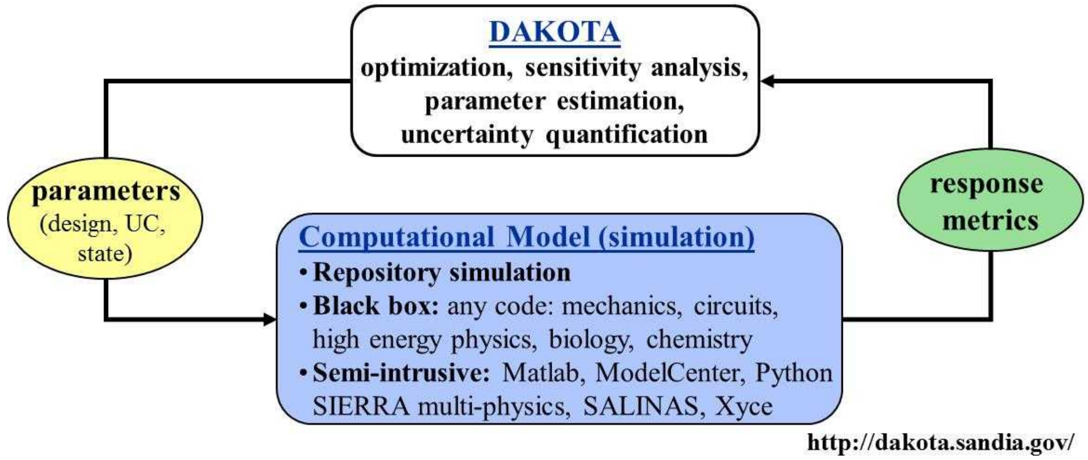

Figure 2-3. DAKOTA Code Workflow and Capabilities

2.1.2.1.2 LIME

This section will describe the LIME capabilities used to support an advanced PA model framework.

LIME (Lightweight Integrating Multi-Physics Environment) (Schmidt et al. 2011) provides a nonintrusive capability for the numerical coupling of multi-physics codes. Specific capabilities include (Figure 2-4):

- Operator-split coupling of legacy software
- Inherit existing QA of legacy software

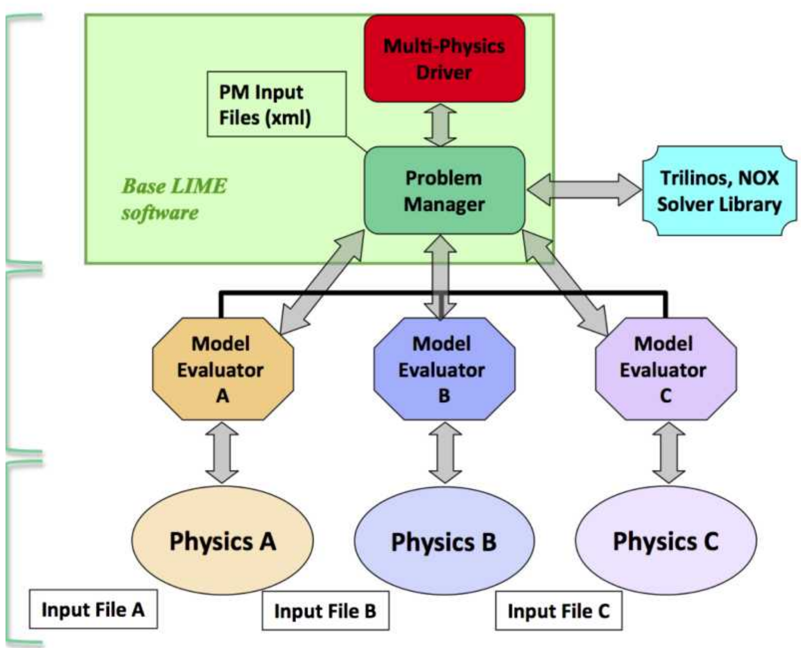

Figure 2-4. LIME Code Workflow and Capabilities

2.1.2.1.3 PFLOTRAN

This section will describe the PFLOTRAN capabilities used to support an advanced PA model framework.

PFLOTRAN is a multi-physics thermal-hydrologic-chemical (THC) simulator that is designed to take advantage of HPC capabilities. PFLOTRAN capabilities and applications are described in Mills et al. (2007), Lu and Lichtner (2007), Hammond et al. (2007; 2008; and 2011), and Lichtner and Hammond (2012). PFLOTRAN has proven useful in tackling challenging subsurface modeling and simulation problems, including the Hanford site (Hammond et al. 2008), and carbon sequestration modeling (Lu and Lichtner 2007).

PFLOTRAN is a massively parallel, multi-phase, multi-component reactive transport code that uses the Portable Extensible Toolkit for Scientific Computation (PETSc) framework as the basis for performing the parallel computations. PFLOTRAN is an open-source code that employs an object-oriented design based mainly on the Fortran 90 and Fortran 2003 languages. The flow and reactive transport capabilities in PFLOTRAN originally were implemented based on structured grids in the PETSc framework. However, recent development has been undertaken to employ structured Adaptive Mesh Refinement to provide high resolution where required, such as in an area in which a contaminant plume must be highly resolved within a large-scale flow and transport domain.

Specific PFLOTRAN capabilities for the simulation of generic disposal systems include:

- Multi-physics
    - Multi-phase flow
    - Multi-component transport
    - Chemical processes
    - Thermal and heat transfer processes
- High-Performance Computing (HPC)
    - Built on PETSc – parallel solver library
    - Massively Parallel
    - Structured and Unstructured Grids
    - Scalable from Laptop to Supercomputer
- Modular design for easy integration of new capabilities

In a generic disposal system model, multi-physics representations are needed for the source term and EBS evolution, EBS and NBS flow and transport, and biosphere transport and receptor uptake. These processes are summarized in Figure 2-5.

For the initial repository demonstration problem, it is expected that PFLOTRAN will be used to simulate the source term/EBS evolution and the EBS/NBS flow and transport. The biosphere will not be simulated. As the conceptual model and computational frameworks evolve, it is expected that independent multi-physics codes for the source term and EBS evolution and for the biosphere will be incorporated. These multi-physics codes will be numerically coupled to the PFLOTRAN-based flow and transport modeling capabilities using LIME.

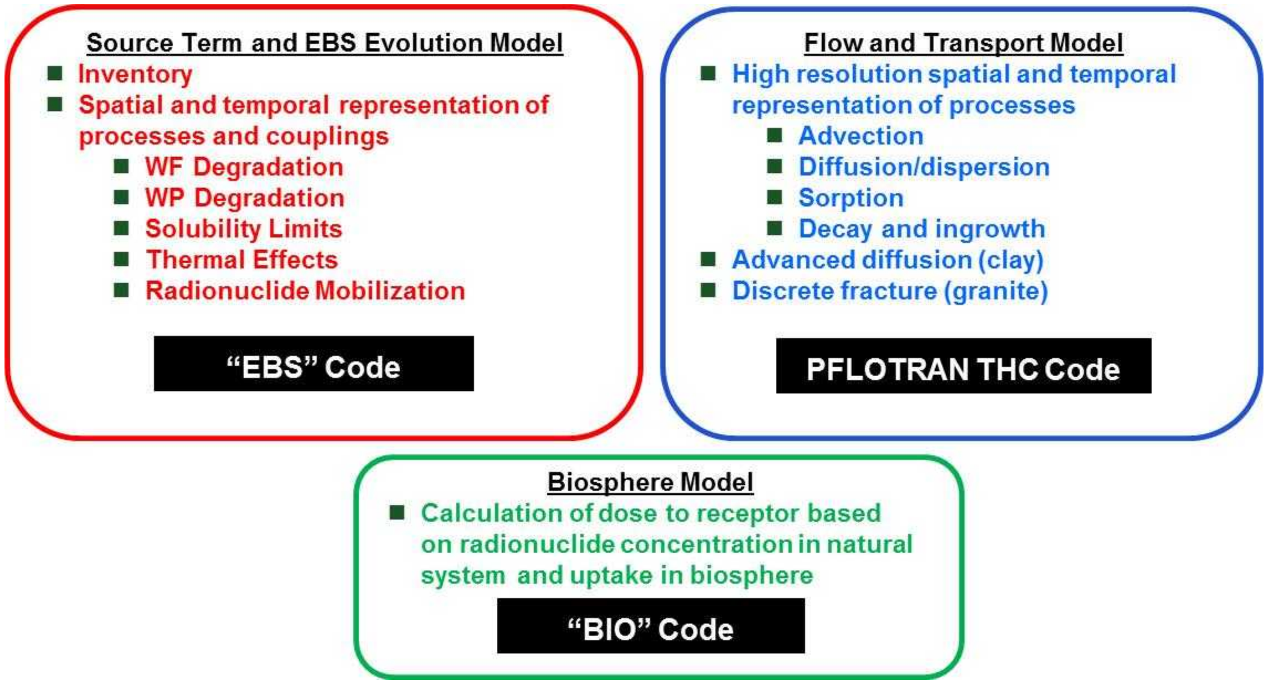

Figure 2-5. Disposal System Integrated Process Models

2.1.2.1.4 Source Term and EBS Evolution

A generic disposal system model must be able to represent the inventory, waste form, and waste package degradation processes contributing to the radionuclide source term.

This section will describe the PFLOTRAN source term and EBS evolution modeling capabilities used in support of the initial generic repository PA model and planned future implementation of a separate source term and EBS evolution code to support an advanced PA model framework.

Specific source term and EBS evolution processes include:

- Waste form degradation (UNF, HLW glass)
  - Radionuclide inventory, including decay chains.
  - PFLOTRAN Implementation: The waste form is defined as a "mineral" with the stoichiometry (i.e., radionuclide components) and density of UNF. The waste form mineral phase is defined to be unstable, i.e., it is specified to have large dissociation constants (log K). The degradation rate of the waste form is controlled by the rate of the dissociation reaction.
- Radionuclide solubility limits
  - Aqueous radionuclides that reach solubility limits precipitate as equilibrium secondary minerals; they can dissolve when aqueous concentrations subsequently fall below solubility limits.
  - Solubility calculations must account for fractional contributions of isotopes (i.e., congruent dissolution)
- Waste package degradation
  - Failure mechanisms and rates (e.g., corrosion rates)

In future iterations, independent multi-physics codes for the source term and EBS evolution will be evaluated and, where necessary, incorporated into the PA model framework.

2.1.2.1.5 Biosphere and Receptor

A generic disposal system model must be able to represent the surface and biosphere processes contributing to the dose to a human receptor resulting from radionuclide releases from the NBS. For the initial generic repository demonstration problem, the biosphere will not be modeled.

This section will describe the planned future implementation of a separate biosphere and receptor code to support an advanced PA model framework.

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 generic repository demonstration problem.

3. SUMMARY AND CONCLUSIONS

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

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