PERFORMANCE ASSESSMENT MODEL DEVELOPMENT METHODOLOGY FOR A BEDDED SALT REPOSITORY

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Recent research by the U.S. Department of Energy on the geologic disposal of high-level radioactive waste and spent nuclear fuel has included development of postclosure safety assessment models that are applicable to a "generic" repository site/design in a variety of suitable host rock media, such as shale/clay, crystalline/granite, and salt. The work described here focuses in greater detail on the generic salt repository concept, and a methodology for development of a salt repository performance assessment (PA) model. Current work has concentrated on several key initial steps in the development of a PA model for a generic salt site: (1) FEPs identification specific to salt host rock, (2) definition of a salt repository "reference case," (3) preliminary FEPs screening based on past salt R&D and safety assessments, (4) specification of quantitative sensitivity analyses and/or reasoned arguments necessary to support FEPs screening, and (5) implications of FEPs screening for PA model construction. The outcome of these initial steps is a methodology that helps define the degree of coupling of physical-chemical processes within the PA model, as well as the fidelity required for characterizing each of these processes in the PA model.

I. INTRODUCTION

The United States (U.S.) currently utilizes a "once-through" commercial nuclear fuel cycle wherein nuclear fuel is only burned once in reactors, after which it is to be permanently disposed as waste in a geologic repository. While significant progress has been made over the last several decades regarding technologies for nuclear waste disposal, experience with the Yucca Mountain Project has illustrated the challenges of siting, characterizing, designing, and licensing a geologic repository for high-level radioactive waste (HLW) and spent nuclear fuel (SNF). To help address these challenges, the U.S. Department of Energy's Office of Nuclear Energy (DOE-NE) conducts scientific research and technology development to enable safe disposal, and temporary storage, of SNF and HLW.[1]

DOE has focused in recent years on "generic" research and development (R&D) targeted toward non-site-specific repositories for a range of disposal concepts that are likely to be viable in the U.S. Within the scope of this generic R&D are activities to design a safety case and an associated safety assessment model for geologic disposal of heat-generating waste in a bedded salt formation. Additional R&D activities are focused on other potential repository concepts for HLW and SNF, including mined repositories in shale/clay and crystalline/granite host rock,[2] as well as deep borehole disposal in crystalline basement rock.[3]

The concept of radioactive waste disposal in salt was recognized by the National Academy of Sciences as early as 1957 when they identified salt as the most promising host rock for high-level waste.[4] Disposal of HLW and SNF in a suitable salt formation is attractive because the material is essentially impermeable, self-sealing, and thermally conductive, and a significant experience base exists from earlier studies. A mined repository in salt could potentially achieve complete containment, with no releases to the environment for the undisturbed scenario, i.e., for the expected evolution scenario that does not have any human intrusions into the repository, such as borehole drilling, and does not encounter any natural disruptive events, such as volcanism.[5]

Of primary concern for any geologic repository, in salt or other media, is a confident demonstration of long-term safety. An appropriate means for documenting the safety of a proposed repository is the internationally accepted vehicle of the *safety case*.[6,7] The work described in the present study focuses on certain aspects of the safety case for a generic salt repository; in particular, on a methodology for development of a quantitative safety assessment model.

Much of the model development methodology described here is centered around features, events, and processes (FEPs) identification and screening for salt host rock, and how this constrains the development of a safety assessment model. A safety assessment model refers to a model (or suite of models) used to predict the quantitative performance of the repository system, with a typical outcome being a set of dose or risk histories spanning the range of uncertainty associated with the input parameters to the model. In the U.S. the term *performance assessment* model or PA model is more commonly used.

II. SAFETY CASE CONTEXT FOR PA MODEL DEVELOPMENT

A *safety case* is a formal compilation of evidence, analyses, and arguments that substantiate and demonstrate the safety, and the level of confidence in the safety, of a proposed or conceptual repository.[6] A safety case also provides the necessary structure for organizing and synthesizing existing knowledge in order to help the repository implementing organization prioritize its future R&D activities toward those that are more important for enhancing confidence. The development of a *safety case* for salt host rock is consistent with DOE-NE's current generic approach to repository research and development. The core of such a safety case would be based on the expected performance of salt host rock for the undisturbed scenario. In particular, because the salt host rock is highly impermeable and resilient to external disturbances, it is expected to effectively isolate the waste without the need for complex and long-lasting engineered barriers. This would reduce repository costs and could potentially simplify performance assessment modeling, thereby adding confidence to the eventual licensing safety case. However, technical questions still must be resolved for the disposal of heat-generating waste, which will drive the complex physical-chemical processes more strongly than cooler waste.[5]

Although the scope of a safety case, and the definitions and terminology used therein, differ somewhat across the various international programs,[6,8,9,10] they all have the same goal of understanding and substantiating the safety of a disposal system. The major elements of any safety case are independent of the host medium and have been defined as:[6,7]

- *Statement of Purpose*. Describes the current stage or decision point within the program against which the current strength of the safety case is to be judged.
- *Safety Strategy*. This is the high-level approach adopted for achieving safe disposal and includes the sub-elements of an overall management strategy; strategies for siting, design, and operations; and a safety assessment strategy.
- *Assessment Basis*. This element comprises the sub-elements of site selection, site characterization, and repository design.
- *Disposal System Safety Evaluation.* This element of the safety case includes two major sub-elements: a preclosure safety analysis and a postclosure performance assessment. It also includes qualitative arguments related to the intrinsic robustness of the site and design.
- *Statement of Confidence and Synthesis of Evidence*. The statement of confidence is based on a combination of safety arguments and analyses, and includes a discussion of completeness to ensure that no important issues have been overlooked.

"Performance assessment is arguably the most important part of the safety case..." (p. 53 of Ref. 11) and includes quantification of the long-term, postclosure performance of the repository, analysis of the associated uncertainties in this prediction of performance, and comparison with the relevant design requirements and safety standards. Such an assessment requires conceptual and computational models based on the relevant FEPs that are or could be important to safety. The determination of which FEPs should be included in the development of conceptual, mathematical, and numerical PA models for an undisturbed generic repository in salt is the primary focus of this paper.

III. PA MODEL DEVELOPMENT

The knowledge base for performance assessments in the U.S. is extensive. For example, the left-hand flow diagram in Fig. 1 illustrates the steps in the iterative performance assessment methodology that was used successfully to certify the Waste Isolation Pilot Plant (WIPP) for defense transuranic (TRU) waste[12,13] and to develop the Yucca Mountain License Application,[14] and has been applied to many other waste disposal projects dating back to the 1970s.[15] The PA Model development work described here focuses primarily on two of the boxes in Fig. 1: "Characterize System" and "Identify Scenarios for Analysis", with the eventual goal of completing activities in the box entitled "Build Models and Abstractions" specific to a generic salt repository.

Although the goal of this PA model development effort is intended to be specific to salt, the resulting model framework and computational framework should be easily adaptable to safety assessments for any geologic medium.[16] Common to repository PA models in any medium are four primary model components (see Fig. 2): inventory and source-term, near-field, far-field, and biosphere. The degree of fidelity required for representing physical-chemical processes in these four PA model components is one of the main aspects of the model development work.[17] It will determined through an iterative process based on a risk-informed set of sensitivity and uncertainty analyses conducted with current and evolving PA models, as well as higher fidelity thermal-hydrologic-mechanical-chemical (T-H-M-C) process models, when necessary (see Sec. III.E).

The right-hand side of Fig. 1 is a more detailed flow diagram of the methodology steps described in this paper to provide an initial basis for PA model construction, and is primarily focused on the disposition of the FEPs with regard to their representation in the PA model. A detailed explanation of the process of FEPs identification, FEPs classification, and FEPs screening, can be found in Sec. 2.2.1 of Ref. 14. Ultimately, FEPs are included or excluded from the safety assessment model based on three major criteria: probability of occurrence, consequence to performance, and specific regulatory guidance. A preliminary screening evaluation in this study was based on consensus judgments of a team of scientists with expertise in performance assessment modeling of the WIPP and Yucca Mountain sites. This evaluation considered only the first two FEPs screening criteria, probability and consequence, since potential site-specific regulatory criteria pertaining to the geologic setting, reference biosphere, and/or receptors are not applicable to a generic site. In general, as illustrated by the left side of Fig. 1, the FEPs evaluation process is iterative, so the preliminary screening judgments will be revisited as additional scientific studies are completed.

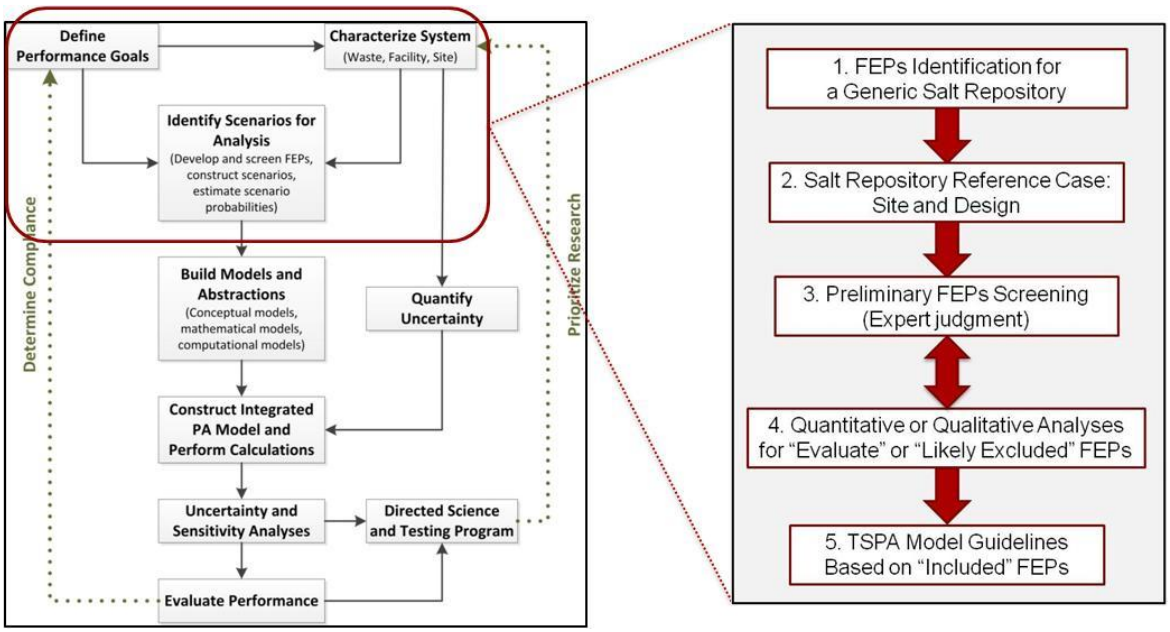

Fig. 1. FEPs Analysis Methodology for Developing a Salt PA Model.

III.A. FEPS Identification

Since the conceptual repository system in this study is assumed to be located in bedded salt, many of the FEPs and associated analyses used for the WIPP performance assessments (e.g., Ref. 12) will be applicable, but subject to some modifications and additions. For example, phenomena caused by decay heat from HLW and SNF will add some FEPs not applicable to WIPP performance assessments, since TRU waste disposed in WIPP generates significantly less heat than HLW or SNF. In addition, the physical and chemical characteristics of HLW are likely to be appreciably different than TRU waste. Therefore, the waste-related FEPs from WIPP will need to be reviewed. Thus, due to the site- and inventory-specific nature of many of the WIPP FEPs, a more general FEPs list[18] was used as the starting point for the preliminary FEPs screening described here, rather than the WIPP FEPs list (App. A of Ref. 5).

Identification of a set of FEPs for a repository system usually begins with a specification of the major physical features of the system, upon which processes and events act. Fig. 2 is a visualization of a generic salt disposal system, divided into a set of components and features, with the major features depicted in a linear fashion from left to right, beginning with the waste form and moving outward toward the Biosphere. In reality, the components are a set of nested regions. For example, the Natural Barrier completely surrounds the Engineered Barrier System on all sides, and radionuclides can be transported from the Engineered Barrier System to the Natural Barrier along multiple flow pathways, although these details are not shown in Fig. 2.

Sevougian et al.[19] identify 208 disposal system FEPs that are potentially relevant to a repository for permanent disposal of SNF and HLW at a generic salt site with the engineered and natural features shown in Fig. 2. Their FEPs are based on the FEP list developed by Freeze et al.[18] for a generic disposal system in any one of four different disposal concepts: mined crystalline/granite, mined shale/clay, mined salt, and deep borehole crystalline. The FEPs list in Freeze et al.[18] was developed from several comprehensive FEP lists and other relevant information.[20,21,22] The resulting FEPs in Freeze et al.[18] were modified by Sevougian et al.,[19] as necessary, to be more specifically relevant to a generic mined repository in bedded salt (Step 1 in Fig. 1). These modifications were in the form of additional or different "Associated Processes" for some of the FEPs (see App. A of Ref. 19).

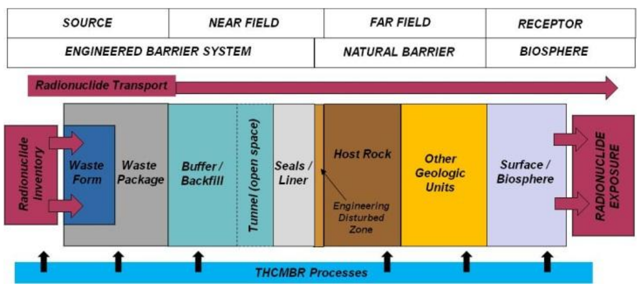

Figure 2. Features and Components of the Generic Salt Disposal System.

III.B. Salt Disposal Reference Case

A safety assessment and the associated PA model typically address a specific site; a well-defined inventory, waste form, and waste package; a specific repository design; and a specific concept of operations. FEPs are then identified and screened in the context of this information. This level of specificity does not exist for a generic site, so it is important to establish a reference site/design, called a *salt disposal reference case* (Step 2 in Fig. 1), to act as a surrogate for site-specific and design-specific information upon which the preliminary FEPs screening judgments may be based (Step 3 in Fig. 1).

This reference site/design for the generic salt repository is discussed in detail in Vaughn et al.[23] and includes a detailed set of assumptions that enable the preliminary FEPs screening to go forward for a generic salt repository. These assumptions are not intended as requirements for the ultimate site or design and, if they are shown to be inappropriate when the final site and design are selected, the FEPs screening will be revisited. The reference case identifies the information needs for preliminary safety assessments, including the relevant information for the Engineered Barrier System (EBS), the Geosphere and Natural Barrier System (NBS), the Concept of Operations, the Biosphere, and the Regulatory Environment (Fig. 3 in Ref. 23). The reference case is intended to contain sufficient information to help focus and guide the direction of the PA model development and parameterization, eventually including a representation of the epistemic uncertainty in parameter values based on the current state of knowledge.[24]

III.C. Preliminary FEPs Screening

After development of a salt-specific FEPs list and a salt repository reference case, the next step is to assign each individual FEP a preliminary screening disposition stating whether it should be included or excluded with respect to a salt PA model (Step 3 in Fig. 1). This preliminary screening disposition is based initially on scientific judgment and will be supported later by documented reasoned arguments or quantitative sensitivity analyses. The preliminary screening in Sevougian et al.[19] was based on five categories:

- Included – A FEP that is almost certain to be screened in to the PA Model, independent of the type of salt site or specific site characteristics. An example of an included FEP is Advective Transport in the Geosphere.
- Excluded – A FEP that is almost certain to be screened out of the PA Model, independent of the specific salt site. An example is Effects of Repository Heat on the Biosphere.
- Site-Specific – A FEP that requires a substantial amount of detailed information for a specific site evaluation. An example is Human Intrusion, which requires knowledge of the potential for mining and resource extraction activities at a specific site in order to develop a detailed screening argument.
- Design-Specific – A FEP that requires detailed information for a specific repository design. An example would be Chemical Effects at EBS Component Interfaces, which requires knowledge of waste package design and EBS materials to formulate a detailed screening argument.
- Evaluate – All other FEPs are candidates for quantitative sensitivity analyses to determine their disposition with respect to the generic salt PA Model. Some of these analyses may involve detailed coupled process models. For example, the hydrologic state at and near the waste package during the initial thermal pulse is likely to result from coupled T-H-M-C processes.

The modifier "Likely" has been added to some of the "Excluded" FEPs, i.e., they are given a preliminary classification of “Likely Excluded,” but require additional analysis to justify their exclusion from the PA model (see Section III.D). Thus, “likely excluded” is similar to “evaluate.” Also, these five categories are not necessarily mutually exclusive because of the broad nature of the original FEPs descriptions, i.e., some aspects of a FEP may likely be excluded while others need to be evaluated, or may even be included.

III.D. Sensitivity Analyses for FEPs Identified as “Evaluate”

Those FEPs identified as “Evaluate” or “Likely Excluded” require further justification regarding their inclusion or exclusion for the generic salt PA Model (Step 4 in Fig. 1), in the form of either qualitative arguments or quantitative analyses. For each of these “Evaluate” or “Likely Excluded” FEPs, Sevougian et al. (App. B of Ref. 19) indicated whether a qualitative or quantitative justification is thought to be most appropriate and provided a brief “reasoned argument” for those that only require a qualitative justification, if such an argument could be expressed succinctly. For FEPs that require a quantitative analysis, those authors identified a preliminary set of sensitivity analyses that could be performed to make a screening decision. This was a set of eleven sensitivity analyses for EBS-related FEPs and three sensitivity analyses for NBS-related FEPs, based on the major physical-chemical processes represented by the associated FEPs: radiological, thermal, mechanical, hydrologic, transport, chemical, or biological processes. (Sensitivity analyses to evaluate nuclear criticality were not considered in this study.)

Although there are more than 75 FEPs that fall into the categories of “Evaluate” or “Likely Excluded,” the number of quantitative sensitivity analyses identified (14) is much less than this because the authors felt that a reasoned argument can be made for excluding most of these FEPs, based on past experience and R&D related to salt repository science and performance assessment.[a] Of those remaining FEPs that cannot be screened based on a reasoned argument, the total number of sensitivity analyses is also less than the number of “Evaluate” or “Likely Excluded” FEPs because multiple FEPs can sometimes be evaluated with single sensitivity analyses.

Many of the identified sensitivity analyses involve multiple physical-chemical processes and therefore are likely to require a coupled process model for the screening calculation. However, in many cases bounding analyses are envisioned to be sufficient. These analyses have conservative values for the key parameters and are simplified in their representation of the key processes and/or simplified in the number of spatial dimensions.

III.E. Guidelines for PA Model Development Based on Included FEPs

A key step in the development of the generic salt PA Model is the identification and evaluation of coupled processes important to overall system performance, and how these coupled processes should be represented in the PA Model in a defensible way. Similarly to FEPs classified as “Evaluate” or “Likely Excluded,” Sevougian et al. (App. C of Ref. 19) have also provided a categorization of “Included” and “Likely Included” FEPs for the PA Model based on the primary physical-chemical process(es): radiological, thermal, mechanical, hydrologic, transport, chemical, or biological. This categorization in terms of major processes allows a grouping of the FEPs into submodels that will form the building blocks of the various domain or component models (e.g., the waste package domain—see Fig. 2) that comprise the generic salt PA Model.

To illustrate how each PA component model can be either derived from the included FEPs or built to ensure that all relevant included FEPs are part of the component model (Step 5 in Fig. 1), the waste package feature/domain (Fig. 2) is used as an example. Based on previous repository modeling experience (e.g., Sections 2.3 and 2.4 of Ref. 14), it is assumed that the primary PA component models needed for the waste package domain are (1) a waste package degradation model, and (2) a radionuclide transport model. The mapping of the included FEPs to these component models is a way of showing: (1) guidelines for the generic salt PA Model construction based on which FEPs (mainly processes) must be part of the PA, and (2) how primary PA component models may be formulated in a hierarchical fashion according to the major physical-chemical processes in the included FEPs. It should be emphasized that this is an illustration that may change depending on the sensitivity of materials and flows to the individual processes and to the time scale of the calculations.

Fig. 3 presents a three-tiered hierarchy of process models to represent waste package degradation in the performance assessment.[b] The “core” of the waste package degradation component model is a coupled thermal-mechanical (T-M) “submodel” to predict the loads on the waste package overpack based on creep closure of emplacement drifts and reconsolidation of

[a] For an eventual licensing case, all exclusion arguments must have some type of quantitative basis that can be documented or referenced.

[b] The submodels required for radionuclide transport in the waste package domain are not discussed here, but may be found in Sevougian et al.[19]

crushed salt backfill surrounding the waste package. Slow viscoplastic flow (creep) of rock salt in the crushed salt backfill is quite temperature dependent, so a T-M coupling is required for these calculations. In effect, the T-M processes are the central "core" of the waste package degradation component model.

A more complete component model must also consider stresses generated by the presence of fluid phases in the pore spaces of the backfill. Thus, as a second tier in the hierarchical construction of the waste package structural model, the effects of hydrologic inflow could be considered. This is important for two reasons. First, if liquid brine completely fills the void space in the crushed salt backfill, it will provide a backpressure that resists further consolidation of backfill. Second, H_2 gas generation from anoxic corrosion of the steel overpack, which is the basis of the third-tier model discussed below, will not occur without the presence of liquid water. The presence of liquid brine could be represented as a fixed or predefined parameter in the core T-M submodel, or could be represented as a coupled thermal-mechanical-hydrologic (T-M-H) submodel, which is illustrated as the second tier in Fig. 3.

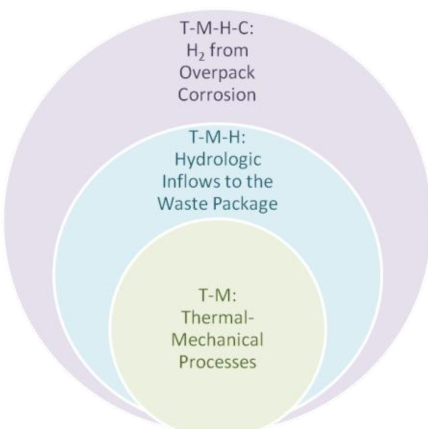

Fig. 3.[19] Hierarchy of coupled submodels for degradation of the waste package.

Anoxic corrosion is important because it can both reduce the thickness of the outer corrosion barrier and it can generate gas that provides a backpressure resisting closure of the emplacement drifts or potentially causing rock fracturing if the generated gas volume is large enough. The presence of gas could initially be represented as a fixed parameter or time history in either the core T-M submodel or in the T-M-H second-tier submodel, or subsequently coupled to a dynamic chemical (C) model of gas generation that is part of a coupled thermal-mechanical-hydrologic-chemical (T-M-H-C) submodel. This T-M-H-C submodel is shown as a third tier in Fig. 3. The second and third tiers in Fig. 3 could be combined if corrosion and hydrologic inflows are both sensitive to the thermal pulse and therefore highly transient. Alternately, the fully coupled T-M-C-H submodel may not be a necessary part of the PA model if gas generation or hydrologic inflows can be approximated or bounded in an appropriate manner. In particular, it is envisioned that coupled processes near the heat-generating waste and in the disturbed rock zone may be included simply as boundary conditions to the PA Model or incorporated as part of the PA model source term, especially if their time scale is short relative to the radionuclide transport time to the biosphere. Information from PA sensitivity and uncertainty analyses, as well as from studies with T-M-C-H process model(s), will be used to make this determination.

The coupled process models in Fig. 3 are based on a subset of the FEPs identified as "Included" and "Likely Included" in Sevougian et al. (App. C of Ref. 19). Table I identifies these included and likely included FEPs that are relevant to structural response of the waste package. The FEPs in Table I have been sorted into a "core" submodel for T-M behavior in the waste package domain, with additional FEPs identified for the T-M-H and T-M-H-C submodels in the second and third tiers, respectively, of Fig. 3.

IV. CONCLUSIONS

Recent research by the U.S. Department of Energy on the geologic disposal of high-level radioactive waste and spent nuclear fuel has focused on development of postclosure safety assessment models that are applicable to a "generic" repository site/design in a variety of suitable host rock media, such as shale/clay, crystalline/granite, and salt. The work described here focuses in greater detail on the generic salt repository concept, and a methodology for development of a salt repository PA model.

Current activities have concentrated on several key initial steps in the development of a PA model for a generic salt site:

- FEPS identification specific to bedded salt host rock
- Definition of a salt repository "reference case"—descriptions and initial and boundary conditions for the natural and engineered systems for a generic bedded salt site
- Preliminary FEPS screening for the reference case based on past salt repository R&D and safety assessments (including the WIPP knowledge base)
- Specification of quantitative sensitivity analyses and/or qualitative reasoned arguments necessary to support FEPs screening

- Implications of FEPs screening for the construction of a generic salt PA model based on the physical-chemical processes in the included FEPs

The result of these initial steps suggests a hierarchical methodology for integration of PA model components that helps define the degree of coupling of physical-chemical processes (e.g., thermal-mechanical-hydrologic-chemical) within the PA model framework, as well as the fidelity required for characterizing each of these processes in the PA system model and its components, such as the dimensionality of the processes and their mathematical representation.

Table I.[19] Included and Likely Included FEPs Related to Submodels for Structural Response of the Waste Package (R = Radiological; T = Thermal; M = Mechanical; H = Hydrologic; C = Chemical)

FEP No.	FEP Description	Notes	R	T	M	H	C
INCLUDED FEPS FOR "CORE" PROCESS SUBMODEL (T-M) FOR STRUCTURAL RESPONSE OF THE WASTE PACKAGE:							
2.1.04.01	Evolution and Degradation of Backfill			✓	✓		
2.1.07.01	Rockfall			✓	✓		
2.1.07.02	Drift Collapse			✓	✓		
2.1.07.03	Mechanical Effects of Backfill	Backfill consolidation around waste package		✓	✓		
2.1.07.04	Mechanical Response of Backfill				✓		
2.1.07.05	Mechanical Response of Waste Packages				✓		
2.1.07.06	Mechanical Response of SNF Waste Form				✓		
2.1.07.07	Mechanical Response of HLW Waste Form				✓		
2.1.07.08	Mechanical Response of Other EBS Components	Waste package support materials only			✓		
2.1.07.09	Mechanical Effects at EBS Component Interfaces				✓		
2.1.11.01	Heat Generation in EBS			✓			
2.1.11.03	Effects of Backfill on EBS Thermal Environment			✓	✓		
2.1.11.04	Effects of Room Closure on EBS Thermal Environment			✓	✓		
2.1.11.06	Thermal-Mechanical Effects on Waste Form and In-Package EBS Components			✓	✓		
2.1.11.07	Thermal-Mechanical Effects on Waste Packages			✓	✓		
2.1.11.08	Thermal-Mechanical Effects on Backfill			✓	✓		
ADDITIONAL INCLUDED FEPS FOR WASTE PACKAGE STRUCTURAL RESPONSE, WITH FLOW (T-M-H):							
2.1.08.01	Flow Through the EBS	Determines brine availability during consolidation				✓	
2.1.08.02	Flow in and Through the Waste Package	Determines presence of water in the waste package				✓	
2.1.08.03	Flow in Backfill	Determines brine availability during consolidation				✓	
2.1.08.08	Capillary Effects in EBS	Determines brine availability during consolidation				✓	
ADDITIONAL INCLUDED FEPS FOR WASTE PACKAGE STRUCTURAL RESPONSE, WITH FLOW AND CORROSION (T-M-H-C):							
2.1.03.02	General Corrosion of Waste Packages	Thickness of waste package overpack		✓		✓	✓
2.1.03.05	Hydride Cracking of Waste Packages	Integrity of overpack when pits/cracks form		✓			✓

ACKNOWLEDGMENTS

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. This paper has been reviewed and approved as SAND2012-10626C.

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