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Challenge Problem and Milestones for: Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Integrated Performance and Safety Codes (IPSC)

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Abstract

This report describes the specification of a challenge problem and associated challenge milestones for the Waste Integrated Performance and Safety Codes (IPSC) supporting the U.S. Department of Energy (DOE) Office of Nuclear Energy Advanced Modeling and Simulation (NEAMS) Campaign. The NEAMS challenge problems are designed to demonstrate proof of concept and progress towards IPSC goals. The goal of the Waste IPSC is to develop an integrated suite of modeling and simulation capabilities to quantitatively assess the long-term performance of waste forms in the engineered and geologic environments of a radioactive waste storage or disposal system. The Waste IPSC will provide this simulation capability (1) for a range of disposal concepts, waste form types, engineered repository designs, and geologic settings, (2) for a range of time scales and distances, (3) with appropriate consideration of the inherent uncertainties, and (4) in accordance with robust verification, validation, and software quality requirements.

To demonstrate proof of concept and progress towards these goals and requirements, a Waste IPSC challenge problem is specified that includes coupled thermal-hydrologic-chemical-mechanical (THCM) processes that describe (1) the degradation of a borosilicate glass waste form and the corresponding mobilization of radionuclides (i.e., the processes that produce the radionuclide source term), (2) the associated near-field physical and chemical environment for waste emplacement within a salt formation, and (3) radionuclide transport in the near field (i.e., through the engineered components – waste form, waste package, and backfill - and the immediately adjacent salt). The initial details of a set of challenge milestones that collectively comprise the full challenge problem are also specified.

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ACRONYMS

CSNF	commercial spent nuclear fuel
CT	Capability Transfer
DOE	Department of Energy
DSNF	DOE spent nuclear fuel
EDZ	excavation disturbed zone
EBS	Engineered Barrier System
ECT	Enabling Computational Technologies
FEP	feature, event, and process
FMM	Fundamental Methods and Models
GTCC	greater than class C waste
HLW	high-level waste
HTGR	high-temperature gas-cooled reactor
IPSC	Integrated Safety and Performance Codes
LTHLW	lower than high-level waste
NE	Nuclear Energy
NEA	Nuclear Energy Agency
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NRC	Nuclear Regulatory Commission
PA	performance assessment
PIRT	phenomena identification and ranking table
SNL	Sandia National Laboratories
SQE	software quality engineering
THCM	thermal-hydrological-chemical-mechanical
THCMBR	thermal-hydrological-chemical-mechanical-biological-radiological
UFD	Used Fuel Disposition
UQ	uncertainty quantification
V&V	verification and validation
VU	verification and validation and uncertainty quantification
WF	waste form
WIPP	Waste Isolation Pilot Plant
WP	waste package
YMP	Yucca Mountain Project

1. INTRODUCTION

The U.S. Department of Energy (DOE) Office of Nuclear Energy (NE) Advanced Modeling and Simulation Campaign co-ordinates the development of Integrated Performance and Safety Codes (IPSCs) in four technical areas: Fuels; Reactors; Safeguards and Separations; and Waste. Within the DOE-NE Advanced Modeling and Simulation (NEAMS) Campaign, challenge problems have been identified as a mechanism to demonstrate proof of concept and progress in each of the four IPSC technical areas. This report describes the specification of a challenge problem and the initial details of a set of associated challenge milestones for the Waste IPSC. The specific details of the challenge milestones are expected to evolve as the Waste IPSC is developed. Changes will be captured through iterations of the Waste IPSC planning and requirements documents, as necessary.

1.1. NEAMS Challenge Problem Overview

Specific criteria for NEAMS challenge problems are:

- Tied to at least one DOE-NE Research and Development Objective
 - *Objective 1:* Develop Technologies and Other Solutions that Can Improve the Reliability, Sustain the Safety, and Extend the Life of Current Reactors
 - *Objective 2:* Develop Improvements in the Affordability of New Reactors to Enable Nuclear Energy to Help Meet the Administration's Energy Security and Climate Change Goals
 - *Objective 3:* Develop Sustainable Nuclear Fuel Cycles
 - *Objective 4:* Understand and Minimize the Risks of Nuclear Proliferation and Terrorism
- A problem stakeholders need to have solved
- Breaks new technical ground
- Computationally demanding and scientifically complex
 - Predictive
 - Couples physical phenomena
- Success can be demonstrated

NEAMS challenge problems also provide a means to:

- Guide NEAMS and Waste IPSC planning and development activities
- Identify, foster, and organize collaborations internal and external to NEAMS
- Deliver incremental capabilities to customers
- Demonstrate measurable progress toward long-term goals to customers and stakeholders
- Discover technical and computational gaps, develop contingencies, and mitigate long-term risks

- Leverage commonalities between the four NEAMS IPSCs and integrate with the NEAMS supporting elements (e.g., Fundamental Methods and Models (FMM), Verification and Validation and Uncertainty Quantification (VU), Enabling Computational Technologies (ECT), and Capability Transfer (CT))
- Define a roadmap for success of the Waste IPSC to deliver on its long-term goals

In addition to the challenge problems, intermediate challenge milestones may be specified to demonstrate incremental progress toward, but not fully address, the challenge problems.

1.2. Waste IPSC Overview

The overarching goal of the Waste IPSC is to develop an integrated suite of modeling and simulation capabilities to quantitatively assess the long-term performance of waste forms in the engineered and geologic environments of a radioactive waste storage or disposal system (SNL 2009, Section 1). This requires the simulation of the coupled thermal-hydrologic-chemical-mechanical-biological-radiological (THCMBR) processes that govern radionuclide (or other hazardous constituent) movement from the waste forms through the engineered components and the geosphere for a range of alternative disposal system designs (e.g., disposal concept, waste emplacement geometry, waste form type, engineered component designs, geologic setting) and conditions (e.g., saturated vs. unsaturated flow, boiling vs. non-boiling temperature, reducing vs. oxidizing chemistry). The simulation of the coupled THCMBR processes is required over a broad range of time scales (nanoseconds to millions of years) and distances (angstroms to kilometers).

To achieve these goals, the Waste IPSC will incorporate three levels of model fidelity: constitutive relationships derived from mechanistic sub-continuum processes; high-fidelity continuum models; and moderate-fidelity performance assessment (PA) models. In addition to directly supporting disposal system simulation, the use of three different levels of fidelity will also support the verification and validation (V&V) and uncertainty quantification (UQ) of the models and their inputs.

To date, the development of radioactive waste disposal system models (both in the U.S. and internationally) has generally been limited to the PA-model level of fidelity (i.e., models rely on approximations and/or surrogate representations of the THCMBR processes and their couplings, often based on empirical relationships), each application has been focused on a very specific disposal system concept/design, and PA-model results have been focused on estimating system-level performance (e.g., dose). These PA models have typically been developed from a set of loosely linked codes, each of which describes a very specific (and often uncoupled) process. As a result, current PA models are not very flexible to changes in designs or disposal conditions and are generally validated for only a narrow range of designs or disposal conditions. The long time scales (>100,000 years) that need to be considered lead to additional difficulties in validating the surrogate models and approximated couplings. A typical consequence of this current PA approach is that significant safety margins (i.e., conservatism) are often necessary to accommodate the model approximations and large uncertainties.

The Waste IPSC will represent a significant advancement beyond current PA models by providing:

- Application Flexibility – The three levels of fidelity of the Waste IPSC will be applicable to a wide range of alternative disposal system designs and for several different objectives. The PA-scale models can be used to estimate system-level performance to support scoping comparisons of alternative disposal concepts, prioritization of activities, and/or licensing. The high-fidelity continuum-scale models can be used to estimate both system-level and subsystem-level performance to support system design and evaluation (e.g., identification of key engineered and geologic system components and phenomena). The sub-continuum-scale constitutive relationships can be used to characterize processes and/or material properties controlling subsystem-level performance (e.g., identification of key material properties for different waste streams and candidate waste forms).
- Improved Technical Defensibility – The coupling among THCMBR processes within and between the engineered and geologic environments will be fully captured, particularly in the high-fidelity continuum models. Model V&V will be in accordance with robust NEAMS-wide criteria and will be supported by cross-fidelity comparisons and integration. Where appropriate (e.g., particularly for processes related to degradation of engineered components, such as waste form dissolution), process models and couplings supporting the Waste IPSC will be based on constitutive relationships derived from mechanistic sub-continuum processes. The constitutive relationships will be upscaled to the high-fidelity continuum models, and further abstracted to PA models. Models will be validated by independent data, where possible, such as physical property measurements, laboratory-scale kinetics measurements, field observations, and archeological and natural analog behavior.
- Advanced Computational Capability – The Waste IPSC will be implemented within an integrated computational framework, in accordance with NEAMS-wide standards. The framework will support a High Performance Computing environment to enable detailed high-fidelity investigations and/or extensive probabilistic evaluations.

There are several potential customers for the Waste IPSC. In the next few years, Waste IPSC development efforts and/or challenge milestones may provide insights on disposal system modeling to the DOE-NE Used Fuel Disposition (UFD) Campaign. The DOE-NE UFD Campaign may, in turn, provide information to the Secretary of Energy's Blue Ribbon Commission (BRC) on America's Nuclear Future. The Waste IPSC will also be used by the DOE-NE Waste Form (WF) Campaign in evaluating the interplay between waste form durability and disposal system performance for various waste forms and disposal system environments. In the next 5-10 years, the capabilities of the Waste IPSC will be needed by the DOE-NE UFD Campaign to inform the implementation of BRC recommendations and evaluate the relative performance and long-term safety of alternative radioactive waste disposal concepts and designs. The Waste IPSC will also inform the DOE-NE WF Campaign about the potential benefits of high performing waste forms for selected waste streams in specific disposal system environments. In that same time frame, simulations enabled by the Waste IPSC capabilities may provide input and insights to the U.S. Nuclear Regulatory Commission (NRC) as they consider revisions to the federal regulations governing radioactive waste disposal. Finally, in the next 20-

50 years, the Waste IPSC will be needed by the DOE to support site selection and to prepare a defensible technical basis (i.e., a PA) for a license application for the selected disposal system alternative(s).

The remainder of this report describes the specification of a Waste IPSC challenge problem and associated milestones that satisfy the NEAMS criteria and demonstrate proof of concept and progress towards these Waste IPSC goals and requirements. Section 2 describes the overall scope of the Waste IPSC and identifies the sub-scope that forms the basis for the challenge problem and the associated challenge milestones. Section 3 outlines the specific challenge milestones. Section 4 provides a summary of the challenge problem and milestones and how they satisfy the NEAMS challenge problem criteria.

2. TECHNICAL AND COMPUTATIONAL SCOPE

In order to identify a reasonable scope for a challenge problem, it is first necessary to understand the scope of the entire Waste IPSC. Section 2.1 summarizes the scope of the Waste IPSC. Section 2.2 then identifies the relevant subset of that scope necessary to specify an appropriate Waste IPSC challenge problem.

2.1. Waste IPSC Scope

2.1.1. Technical Scope

As described in Section 1.2, the Waste IPSC will provide the capabilities to quantitatively assess the long-term performance of waste forms in the engineered and geologic environments of a radioactive waste storage or disposal system, using mathematical representations of the coupled THCMRB processes that govern radionuclide (or other hazardous constituent) movement through the entire disposal system. The Waste IPSC will enable simulation of disposal system performance at three different model fidelities for a range of candidate waste forms, disposal concepts and designs, engineered and geologic environments, and associated conditions over a broad range of time and length scales. The multi-fidelity development of the Waste IPSC will incorporate capabilities for (1) characterizing material properties (e.g., chemical reactions and chemical kinetics) at the sub-continuum scale, (2) upscaling into constitutive equations at the continuum scale, (3) developing high-fidelity models of coupled THCMRB processes (e.g., reactive transport), and (4) abstracting the coupled processes into computationally efficient PA models for quantitative assessment of disposal system performance.

In collaboration with the DOE-NE Used Fuel Disposition (UFD) Campaign (Freeze et al. 2010, Section 2.1), a set of 6 potential waste form type groupings (Table 2-1) and 8 potential disposal concept/geologic setting groupings (Table 2-2) were identified to define the expected range (based on current knowledge) of disposal system concepts, designs, settings and conditions.

Table 2-1. Groupings of Potential Waste Form Types

Group Number	Waste Form Type	Description
1	Used Nuclear Fuel (UNF)	e.g., Commercial, DOE-Owned, HTGR
2	High-Level Waste (HLW) Glass	Current (e.g., borosilicate) and future (e.g., no minor actinides)
3	High-Level Waste (HLW) Glass Ceramic / Ceramic	Current (glass bonded sodalite) and future (e.g., from electrochemical processing)
4	High-Level Waste (HLW) Metal Alloy	From electrochemical or aqueous reprocessing, cermets
5	Lower Than HLW (LTHLW)	Class A, B, and C, and GTCC
6	Other	Molten salt, electro-chemical refining waste, etc.

Note: HTGR = High-temperature gas-cooled reactor; GTCC = Greater than Class C.

Table 2-2. Groupings of Potential Disposal Concepts and Geologic Settings

Group Number	Disposal Concept / Geologic Setting	Description
1	Surface Storage	Long-term interim storage at reactors or at centralized sites
2	Shallow Disposal	e.g., near-surface disposal, LTHLW sites (Depths <= 100 m)
3	Mined Geologic Disposal (Hard Rock, Unsaturated)	Granite/crystalline or tuff (Depths > 100 m)
4	Mined Geologic Disposal (Hard Rock, Saturated)	Granite/crystalline or tuff (Depths > 100 m)
5	Mined Geologic Disposal (Clay/Shale, Saturated)	Clay/shale (Depths > 100 m)
6	Mined Geologic Disposal (Salt, Saturated)	Bedded or domal salt (Depths > 100 m)
7	Deep Borehole Disposal	Granite/crystalline (Depths~ 1000 m)
8	Other	Sub-seabed, carbonate formations, etc.

The groupings in Table 2-1 and Table 2-2 are described in more detail in Freeze et al. (2010, Sections 2.1.1 and 2.1.2). These groupings result in 35 combinations (ignoring the placeholder “Other” groups) of waste form types and disposal concepts/geologic settings that broadly define the range of potential alternative disposal system designs that might need to be evaluated using the Waste IPSC. Within any single alternative disposal system design there may be important sub-designs (e.g., waste emplacement geometry, thermal loading, engineered component design and materials) and/or conditions (e.g., saturated vs. unsaturated flow, boiling vs. non-boiling temperature, reducing vs. oxidizing chemistry) that may further delineate the range of technical capabilities required of the Waste IPSC. As technologies and socio-political drivers evolve, these waste form and concept/setting groupings may also evolve.

To develop a conceptual understanding of the design components, physical domains, and phenomena that may be potentially relevant to these 35 disposal system alternatives, and therefore need to be encompassed by the Waste IPSC modeling and simulation capabilities, it is useful to identify the key common system components and phenomena. Figure 2-1 shows a conceptualization of a generic disposal system that includes components, domains, and phenomena common to most of the 35 disposal system alternatives.

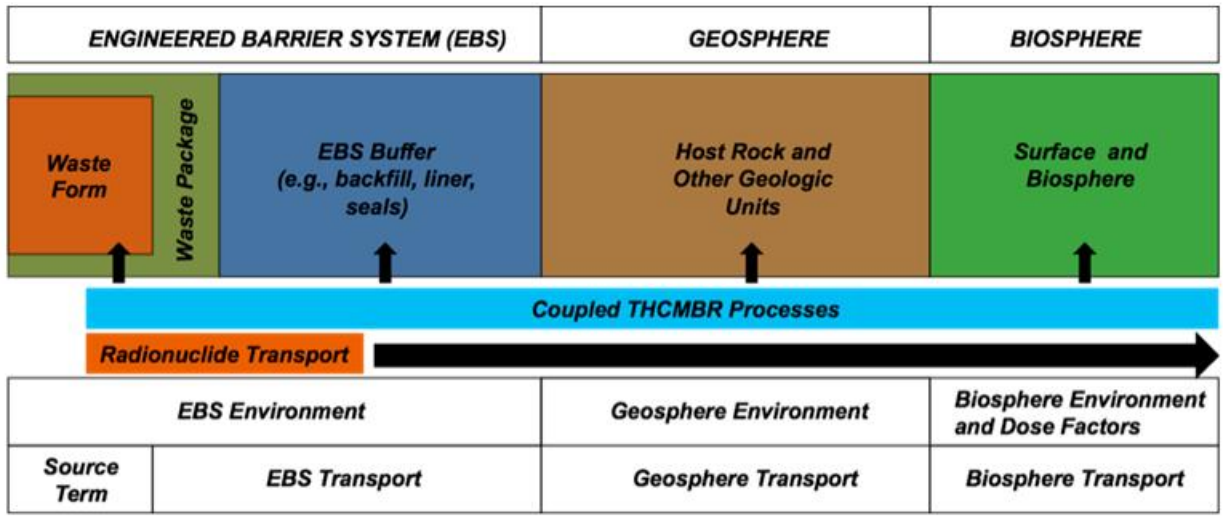


Figure 2-1. Components of a Generic Disposal System.

The top half of Figure 2-1 shows the physical domains of the generic disposal system. The generic system contains three domains: the engineered barrier system (EBS), the geosphere, and the biosphere. Each of these three domains contains sub-domains: waste form, waste package, and buffer for the EBS; host rock and other geologic units for the geosphere; and the land surface for the biosphere. The bottom half of Figure 2-1 shows the phenomena that can affect each of these domains and sub-domains. These phenomena include, at a high level, the coupled THCMRB processes that describe (1) waste form degradation and the source term, (2) radionuclide transport through the EBS, (3) radionuclide transport through the host rock and surrounding geologic units (i.e., the geosphere), and (4) radionuclide transport, uptake, and health effects in the biosphere. In addition to their direct effects on radionuclide transport, the coupled THCMRB processes also influence the physical and chemical environments in the EBS, geosphere, and biosphere, which in turn affect water movement, degradation of EBS components, and radionuclide transport.

The terms near field (or near-field environment) and far-field (or far-field environment) are also commonly used to describe the physical domains of a disposal system. The near field encompasses the EBS and well as the interface with, and adjacent portion of, the host rock that experiences durable (but not necessarily permanent) changes due to the presence of the repository (e.g., hydro-mechanical alteration due to tunnel excavation, thermal-chemical alteration due to waste emplacement). The far field encompasses the remainder of the geosphere and the biosphere.

The coupling between THCMRB processes is particularly important in the near field (e.g., reactive transport is likely a key coupled near-field process) due to proximity to the emplaced waste and the induced thermal and chemical gradients. The Waste IPSC modeling and simulation capabilities will aim to incorporate full THCMRB coupling in all domains. However, the degree of coupling required in each domain will be evaluated as the Waste IPSC is developed.

The physical domains and phenomena in Figure 2-1 are presented at a very high level. Additional detail regarding the technical scope of the Waste IPSC can be identified through an analysis of generic disposal system features, events, and processes (FEPs). A FEP generally encompasses a single phenomenon; typically it is a process or event acting upon a feature. FEP analysis includes FEP identification, FEP screening, and FEP implementation. FEP identification can be done at a coarse level of detail such that it is potentially applicable to a broad range of disposal concepts, designs, and geologic settings. However, FEP screening (determination of which FEPs should be evaluated in a model, based on relevance and importance) and FEP implementation (method and level of detail of quantification in a model) must consider the specific disposal system alternative and also the performance metric of interest (e.g., dose, radionuclide concentration, cumulative release, etc.). FEP implementation is further dependent on the model fidelity. FEP analysis is an iterative process that evolves as new information (e.g., experimental data, model results) becomes available.

The Nuclear Energy Agency (NEA) has compiled an international database of FEPs, containing independent disposal system FEPs from several countries (NEA 1999; NEA 2006). Additional information describing FEP analysis methodology, and specific FEP identification for the Yucca Mountain Project (YMP), is available in YMP reports (BSC 2005; SNL 2008). In collaboration with the DOE-NE UFD Campaign, a preliminary set of FEPs potentially relevant to the scope of the Waste IPSC was identified (Freeze et al. 2010, Sections 1 and 2.3). These Waste IPSC FEPs were developed based on the following information:

- Approximately 1,650 FEPs from 10 different national radioactive waste disposal programs contained in the NEA FEP list (NEA 1999, Appendix D; NEA 2006). The NEA FEPs cover a wide range of disposal system designs and geologic settings, but contain considerable redundancy as the same FEP is often identified 10 different times (once by each program).
- 374 FEPs from the YMP FEP list (SNL 2008, Table 7-1). The YMP FEPs are specific to the YMP design concept in an unsaturated, fractured tuff. The NEA FEPs were considered in the development of the YMP FEP list.
- The Phenomena Identification and Ranking Table (PIRT) list developed for the Waste IPSC as part of FY09 planning (SNL 2009, Section 3). A list of 92 Waste IPSC PIRTs were developed from the NEA FEPs and the YMP FEPs, but were limited to a generic EBS domain.

The consolidation and generalization of these FEPs into a set of Waste IPSC FEPs more broadly applicable to a range of disposal alternatives is described in Freeze et al. (2010, Section 2.3). The resulting set of 208 preliminary Waste IPSC FEPs are listed in Appendix A (Table A-1). Each FEP is defined by a “Description” at a broad level of detail such that it is potentially applicable to the full range of disposal system alternatives. Each FEP is further defined by additional details under “Associated Processes”. The FEPs are organized in accordance with a Waste IPSC FEP categorization scheme that is similar to the NEA categorization scheme (NEA 1999, Section 3). The Waste IPSC categorization scheme, illustrated schematically in Figure 2-2, is based on a set of generic domains (features) that are present in most disposal system concepts. Note that the generic features in Figure 2-2 are subsystem components (i.e., additional

details) of the three physical domains (EBS, Geosphere, Biosphere) in Figure 2-1. Figure 2-2 also illustrates how each of the generic features can be acted upon by events (i.e., External Factors) and/or THCMBR processes and indicates the Assessment Basis FEPs that govern the model calculations.

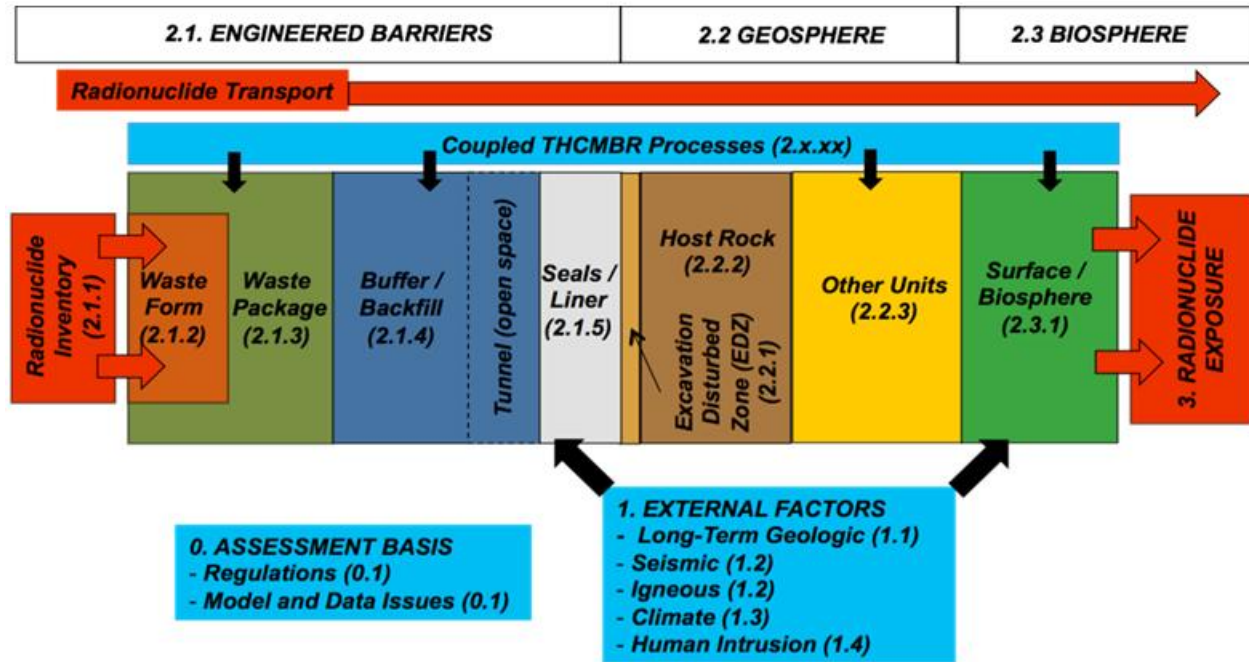


Figure 2-2. Categorization of Features, Events, and Processes (FEPs) in a Generic Disposal System.

Another key aspect of the Waste IPSC categorization scheme is a hierarchical FEP numbering system that groups similar FEPs together. The numbers associated with various domains, features, events, and processes in Figure 2-2 correspond to the FEP numbering system. Across the disposal system domains there is a consistent structure and numbering scheme for the features (2.x.01 contains the first feature, 2.x.02 contains the second feature, etc.) and the processes (2.x.07 contains mechanical processes, 2.x.08 contains hydrologic processes, etc.).

In summary, the technical scope of the Waste IPSC must be broad enough to represent the range of potentially relevant phenomena (and associated time- and length-scales of interest) captured by the 208 FEPs for a range of disposal system alternatives encompassed by the 35 combinations of concepts/settings and waste form types.

To facilitate an evaluation of a specific disposal system design, or a comparison of disposal system alternatives, the Waste IPSC will produce several system and subsystem performance measures (model outputs) as a function of time and location. System-level performance measures may include: human health effects in the biosphere (e.g., annual dose); cumulative radionuclide release to the biosphere; and radionuclide concentrations in the biosphere.

Subsystem-level performance measures may include: radionuclide mass flux and cumulative release across intermediate domain boundaries; radionuclide concentrations within domains; radionuclide mass in place (within domains and remaining in the waste form); engineered component degradation rates; and spatial distributions of various physical and chemical properties (e.g., pH, temperature, fluid saturation, chemical concentrations, dissolution and precipitation rates).

In addition, the Waste IPSC will facilitate the design of waste forms for specific performance targets (i.e., materials-by-design). The evaluation of the radionuclide source terms for different waste streams and candidate waste forms (see Table 2-1) will, in principle, depend on mechanistic sub-continuum processes. The capability to abstract the governing equations for radionuclide release from the various candidate waste forms will require methods for evaluating chemical reactivity and diffusivity of the waste form materials as a function of ambient conditions and material environment. The quantitative assessment of waste form performance in candidate disposal concepts and geologic settings (see Table 2-2) would produce meaningful figures of merit for the desired qualities in a waste form material design.

2.1.2. Computational Scope

The technical scope of the Waste IPSC is supported by and integrated with computational capabilities. These computational capabilities and associated considerations relevant to the Waste IPSC are:

- Verification and Validation: code verification; model validation (over the range of disposal system alternatives, time- and length-scales, model fidelities); upscaling from sub-continuum scale processes to continuum scale processes; availability of validation data and natural analogues
- Uncertainty Quantification: treatment of aleatory uncertainty; treatment of epistemic uncertainty; propagation of uncertainty through the model; model calibration; sensitivity analysis; availability of input data
- Framework Architecture: THCMR multi-physics coupling; inter-fidelity coupling; analysis workflow (including input pre- and post-processing and visualization)
- Software Engineering Environment: software quality; configuration management; data management; software integration

General considerations for each of these computational capabilities in the Waste IPSC are outlined in SNL (2009). These computational capabilities are inter-related with each other, and many are also inter-related with the technical considerations. These inter-relationships are generally identified and addressed through the specification of use cases (SNL 2009, Section 5).

In general, the computational capabilities will be developed concurrently with the technical scope. The computational capabilities that are more inter-related with the technical scope (e.g., upscaling, UQ, and coupling) will be developed with a higher degree of integration, while the

others may be developed more independently. The development of the Waste IPSC computational capabilities will be supported by the NEAMS FMM, VU, ECT, and CT elements.

The final integration of the technical and computational scope will produce a Waste IPSC that (1) is based on mechanistic and predictive constitutive relationships derived from sub-continuum processes, (2) employs fully coupled THCMBR process models, (3) incorporates robust (VU-assessed) V&V and UQ approaches, (4) implements best practices of software quality engineering (SQE), and (4) functions in a high-performance computing environment. These advanced modeling and simulation techniques will produce a Waste IPSC that can be used to simulate the wide range of system designs and conditions demanded by the Waste IPSC.

2.2. Challenge Problem Scope

To demonstrate proof of concept and progress in the Waste IPSC, a challenge problem and associated challenge milestones have been specified. The challenge problem and milestones are a subset of the full scope of the Waste IPSC described in Section 2.1.

2.2.1. Technical Scope

The challenge problem will include the coupled thermal-hydrologic-chemical-mechanical (THCM) processes that describe (1) waste form degradation and the associated mobilization of radionuclides (i.e., the processes that produce the radionuclide source term) and (2) radionuclide transport through the near field. The challenge problem will also include the effects of coupled THCM processes on the physical and chemical environment in the near field. As described in Section 2.1, the near field includes both the EBS components (i.e., waste form, waste package, backfill) and the adjacent portion of the host rock that experiences durable changes due to the presence of the repository. The challenge problem will focus on a specific waste form type from Table 2-1, HLW borosilicate glass, and a specific disposal concept/geologic setting from Table 2-2, mined geologic disposal in salt. This challenge problem disposal alternative captures some of the more complex waste form degradation and mechanical phenomena. The resulting conceptual framework should be readily adaptable to many of the other disposal alternatives.

Model outputs for the challenge problem will include: radionuclide mass flux and cumulative release (out of the EBS and across sub-domain boundaries); radionuclide mass in place (within the waste form (WF), waste package (WP), EBS, and near-field portion of the host rock); and spatial distributions of various physical and chemical properties in the EBS (e.g., pH, temperature, fluid saturation, chemical concentrations, glass degradation rate).

The development of Waste IPSC capabilities to address this challenge problem is expected to take several years. Therefore, the Waste IPSC process models and couplings supporting the challenge problem will be developed, tested, and applied incrementally, with additional capabilities and/or couplings being added in successive phases. The capabilities added during each successive development phase generally build upon, and are coupled to, the previous capabilities. The development phases are defined conceptually as a set of challenge milestones that collectively comprise the full challenge problem. Progress towards these milestones will

provide an indication of intermediate progress towards completion of the entire challenge problem.

The specification of the challenge milestones derives from the key challenge problem conceptual model components:

- Development of THCM process models in each of the physical domains relevant to the challenge problem
 - Source term (borosilicate glass waste form degradation, waste package degradation, radionuclide solubility)
 - Near-field environment (temperature, fluid chemistry, biology, mechanical degradation of EBS components (salt backfill, tunnel closure due to salt creep, EDZ))
 - Near-field transport (advection, dispersion, and sorption of dissolved radionuclides)
- Coupling of the THCM process models within and between domains

These conceptual model components will be developed at both the high-fidelity continuum scale and at the moderate-fidelity PA scale. Where appropriate (e.g., for waste form dissolution), the high-fidelity continuum models and/or the moderate-fidelity PA models will be supported by constitutive relationships developed with support from sub-continuum models and available experimental data, both to aid in defining the functional forms of the constitutive laws and to populate parameters within those constitutive models. Conceptual model development will be supported by the NEAMS FMM supporting element and by the DOE-NE WF Campaign.

Five specific challenge milestones are identified in Table 2-3 to demonstrate the development of the key Waste IPSC conceptual model components listed above at multiple model fidelities. Table 2-3 identifies the degree of THCM coupling desired for each of the process models (i.e., source term, near-field environment, near-field transport). Strong coupling means two-way feedback between processes is desirable, weak coupling means that it is acceptable to approximate or ignore some aspects of the coupling between processes. Table 2-3 also identifies the expected computational capabilities (i.e., level of complexity and integration of V&V, UQ, and SQE tools and frameworks). Further discussion of the computational scope in the challenge milestones is provided in Section 2.2.2.

Table 2-3. Waste IPSC Challenge Milestones

No.	Milestone	Source Term ¹	Near-Field Environment ¹	Near-Field Transport ¹	Computational Capabilities ²
1	Chemical Equilibrium Calculation (for concentrated electrolyte solutions)	T=C	T=C	N/A	Low
2	Waste Form and Waste Package Degradation (for HLW borosilicate glass)	T=H=C=M	T=H=C	N/A	Medium
3	Tunnel Closure (Salt Creep)	N/A	T=M-H	N/A	Medium
4	Heat and Fluid Movement in the Near Field (in a salt repository)	N/A	T=H=C	N/A	Medium
5	Radionuclide Mobilization and Transport in the Near Field (in a salt repository)	T=H=C=M	T=H=C=M	T=H=C=M	High

¹ Strong multi-physics coupling is represented by =; Weak multi-physics coupling is represented by –

² Degree to which computational capabilities outlined in Section 2.1.2 are implemented in milestone

Each of the challenge milestones is discussed in more detail in Section 3. The detailed descriptions include discussions of physical processes and couplings, model implementation, code capabilities to be demonstrated, V&V needs, and data needs. In addition to the detailed descriptions in Section 3, the potentially relevant FEPs for each challenge milestone are identified in Table A-1. The FEPs for each challenge milestone provide an indication of the scope that augments the detail presented in Section 3.

While the final scope of the Waste IPSC will include coupled THCMBR processes (see Section 2.1.1), the coupling of biological and radiological processes (the BR component of THCMBR) are not explicitly identified in Table 2-3 or in any of the challenge milestone descriptions in Section 3. Table A-1 identifies specific biological processes (e.g., FEPs 2.1.03.06, 2.1.10.01, and 2.1.11.13) and radiological processes (e.g., FEPs 2.1.13.01, 2.1.13.02, and 2.1.13.03) that are potentially relevant to the challenge milestones. However, the implementation of these processes in the challenge milestones will be indirect; the effects of biological processes (e.g., microbial activity) will be captured within the effects of other chemical processes, and the effects of radiological processes (e.g., radiolysis, radiation damage) will be captured within the effects of other chemical and mechanical processes. Therefore, the challenge milestones are focused on THCM couplings.

The set of FEPs to be addressed collectively by the five challenge milestones are a subset of the full set of 208 FEPs, with non-relevant FEPs identified as “N/A” in Table A-1. It should also be noted that the subset of FEPs relevant to this challenge problem are only addressed for one of the 35 disposal system alternatives (i.e., HLW borosilicate glass waste form in a mined geologic disposal system in salt). However, the conceptual models and couplings developed for this challenge problem will provide insights, and can be readily extended as appropriate, to other disposal system alternatives.

Finally, just as the disposal alternatives and the FEPs may evolve, so may the milestones, or at least specific details of the milestones. For example, this challenge problem does not include radionuclide transport through the far field geosphere, or radionuclide transport and health effects in the biosphere. However these processes could be incorporated into the challenge problem if necessary.

2.2.2. Computational Scope

As noted in Section 2.1.2, the computational scope (V&V, UQ, SQE tools and frameworks) will be developed in parallel with the technical scope for the Waste IPSC. However, because the full integration of the technical and computational scope in the final Waste IPSC will not occur until after this challenge problem is complete, the challenge milestones will only include partial implementations of some of the computational capabilities, with a focus on the more inter-related capabilities (e.g., upscaling, UQ, coupling).

Within each of the detailed challenge milestone descriptions in Section 3 there are explicit specifications related to UQ, coupling, and, where relevant, to upscaling. There are also explicit specifications of V&V and data needs. During each of the milestone phases, the state of the computational capabilities and its integration with the technical scope will be evaluated. Advancements in computational capabilities will be made with each successive milestone, as shown in Table 2-3.

3. DESCRIPTION OF INDIVIDUAL CHALLENGE MILESTONES

This section provides additional details for each of the five challenge milestones identified in Table 2-3. These five challenge milestones contribute to the solution of the overarching challenge problem of the degradation of HLW borosilicate glass waste form and the associated mobilization and transport of radionuclides through the near-field environment of a disposal system located within a salt formation. The near field includes both the EBS components (i.e., waste form, waste package, backfill) and the adjacent portion of the host rock that experiences durable changes due to the presence of the repository.

The detailed specifications include discussions of physical processes and couplings, model implementation, code capabilities to be demonstrated, V&V needs, and data needs. These specifications are augmented by the list of potentially relevant FEPs in Table A-1. Potentially relevant FEPs are identified for each of the five challenge milestones. The specifications and potentially relevant FEPs for each of the challenge milestones collectively comprise the requirements for the overarching challenge problem.

The computational scope for each challenge milestone is not explicitly identified. However, issues related to V&V, UQ, and coupling are discussed within the details of each of the challenge milestone and issues related to upscaling are discussed within Challenge Milestone 2.

The milestone specifications are presented here at a reasonably high level of detail. More specific details will be identified and planned at the initiation of activity for each milestone.

3.1. Challenge Milestone 1: Chemical Equilibrium Calculation

3.1.1. Description

Physical Processes and Couplings

The water chemistry within the EBS is dependent on the waste form and waste package degradation processes and on the water chemistry in the host rock. The water chemistry in the EBS can be calculated by explicitly accounting for a representative chemical composition of incoming water, the chemical components added to the solution through chemical reactions (e.g., corrosion of waste form and waste package materials), and the equilibrium within and among the coexisting aqueous, gaseous, and solid phases. In a high ionic strength environment, such as in a salt repository, the calculation of activity coefficients of each chemical species must be corrected for specific ion interactions. The chemical equilibrium calculations in this milestone will be based on thermodynamic data for concentrated electrolyte solutions (representative of a high ionic strength environment) over the range of temperatures and chemical compositions considered applicable to the water chemistry in the EBS and host rock of a disposal system in a salt formation.

Model Implementation

High-Fidelity Continuum Model and Performance Assessment Model: In both the high fidelity and PA models, the chemical equilibrium calculation will be implemented in a self-contained code module, which will calculate the concentration of each dissolved or gaseous species and the

amount of each mineral precipitated from the solution for a specified pressure and temperature condition, given the total mass of each chemical component. For a concentrated electrolyte solution, the activity of each dissolved chemical species will be calculated with a Pitzer or specific ion interaction formulation. This code module must be robust so that a solution can be obtained at each spatial node and each time step in the calculation. A key issue is the completeness and self-consistency of thermodynamic database. A large gap exists in data availability, especially at high temperatures for some important radionuclides. For the PA model, the module will be used to systematically evaluate the impact of the uncertainties in thermodynamic data on radionuclide solubility calculations.

3.1.2. Code Capabilities to be Demonstrated

High-Fidelity Continuum Code Capabilities

- Equilibrium calculations for multiphase (aqueous, gaseous, and solid) systems at specified pressure and temperature conditions
- Computation of the activity coefficients of aqueous species and the activity of water in highly concentrated solutions using the Pitzer formulism
- Surface complexation/ion exchange calculations
- Equilibrium calculations involving mineral solid solutions

Performance Assessment Code Capabilities

The same capabilities will be implemented as the high fidelity model. In addition, the PA code will:

- Systematically evaluate the effect of uncertainties in thermodynamic data on radionuclide solubility

3.1.3. V&V Needs

- Pitzer tests cases for equilibrium speciation and reaction path calculations
- Non-Pitzer test cases for equilibrium speciation and reaction path calculations
- Test cases to evaluate the implementation of mass balance calculations as defined by basis species or chemical components
- Test cases to evaluate speciation calculations taking into account solid solution in minerals and mass transfer calculations in a fluid-centered (open system) mode
- Tests of radionuclide solubility calculations against experimental measurements, especially in high ionic strength media and at elevated temperatures

3.1.4. Data Needs

- Thermodynamic data for solid phases and aqueous speciation as well gaseous species, especially the binary or ternary interaction coefficients
- Pitzer parameter data (a Pitzer database)
- Experimental measurements of radionuclide solubility in high ionic strength media and at elevated temperatures

3.2. Challenge Milestone 2: Waste Form and Waste Package Degradation

3.2.1. Description

Physical Processes and Couplings

Waste packages emplaced in a repository will degrade due to stress or chemical corrosion, leading to dissolution of the HLW borosilicate glass waste form and consequent release of radionuclides. As water flows through a degraded (e.g., breached or failed) waste package, the borosilicate glass and internal waste package materials will also degrade. Water inside the waste package may experience a complex set of phase transitions including evaporation, boiling, and condensation. As a result, the overall chemical composition, mineral phases, hydrologic properties, and physical configurations of the materials will evolve with time. Radionuclides mobilized from the waste form degradation processes will be transported away from the waste package by advection or diffusion.

Model Implementation

For both the high-fidelity and the PA models, the codes will calculate radionuclide release from a single failed waste package as a function of water flow and water chemistry, degradation kinetics of the borosilicate waste form and the waste package materials, and the physical configuration of the waste package. This milestone will be developed in stages that deliver sequentially improved materials models as sub-continuum-developed chemical processes and parameters augment and replace phenomenological models. This will be dependent upon success in upscaling atomistic processes to effective constitutive models.

High-Fidelity Continuum Model: In the high-fidelity model, the waste package will be represented using a 3-D high resolution mesh to capture the spatial heterogeneity of the materials inside the waste package. Detailed waste package failure mechanisms (e.g., stress corrosion cracking) will be included in the model. These high-fidelity simulations will invoke constitutive models with associated material property databases, founded on chemical processes that have been identified and quantified by atomistic-scale simulations and experiments. These atomistic chemical processes, including reactions and diffusion, will be aggregated to derive averaged rate laws for glass dissolution, with a process and dataflow that is verified and validated (V&V) and that propagates uncertainties.

Performance Assessment Model: In the PA model, the waste package will be represented as a well-mixed cell or a small number of physically connected compartments. The PA model will be focused on uncertainty quantification through stochastic sampling of input parameter distributions and multiple realizations of waste package degradation.

Upscaling

For this challenge milestone, constitutive relationships describing waste form and waste package material behavior will be derived from mechanistic sub-continuum processes and then upscaled to the high-fidelity continuum model. The accuracy of the high-fidelity simulations, and associated uncertainties, will be limited fundamentally by the fidelity of the underlying constitutive models used to calculate the release rate and reactive transport of radionuclides from

a degrading waste form. Existing models for glass waste form dissolution presuppose an assumed release rate or embody empirically-derived rate equations, which limits their predictive usefulness and increases the uncertainty in those approaches. Large uncertainties in the modeling approach can lead to overly conservative (and expensive) designs of the waste packages and engineered barrier systems to achieve adequate estimates of radionuclide isolation. To enhance the predictive capability of this approach, the constitutive models will be built on a fundamental mechanistic understanding of the chemical and transport processes (starting at the atomistic scale) rather than solely on empirical data. To accomplish this goal, a solution to the upscaling problem will be developed by addressing how to aggregate the discrete atomic chemical processes (reactions that modify the materials and diffusion that underlies chemical transport) into constitutive rate laws, thermodynamic properties, and mechanical properties at the macroscopic scale. This will include the quantitative propagation of uncertainties in the data from the finer (e.g., sub-continuum) scale to the coarser (e.g., continuum) scale of simulation.

The development and implementation of upscaling methods will be systematically constructed via careful formulation of interim steps within the challenge milestone of borosilicate glass dissolution. These steps will define, scope, and implement specific V&V and UQ capabilities in well-controlled, quantifiable systems. This stepwise approach is also intended as a sequence of feasibility studies for various aspects of the upscaling method: develop V&V and UQ procedures in each stage of the upscaling process, identify and fill important gaps in the simulations capabilities and experimental knowledge, and delineate efficiently any potential unanticipated bottlenecks that do not appear tractable. If difficulties arise, workable contingencies could be developed that allow the challenge milestone to be met with more empirical or phenomenological descriptions.

Many of the computational tools (e.g., quantum chemistry methods such as density functional theory, or classical molecular dynamics) necessary to model the relevant chemical phenomena exist. However, some capabilities will likely need further assessment and refinement or new tools may need to be developed. It is anticipated that these improvements will be done in coordination with the NEAMS FMM supporting element. Mathematical techniques and computational methods to perform statistical aggregation of microscopic phenomena, e.g. targeted Monte Carlo techniques, will almost certainly need development, particularly to conform to the requirement that these aggregations propagate UQ through this upscaling.

It is further anticipated that constitutive models based on first principles will only become available after the design and implementation of the high-fidelity codes has started. Therefore, in addition to the development of methods for aggregating sub-continuum phenomena into collectively averaged rate-laws for dissolution, work will also proceed at the continuum scale downwards. Such work may include developing alternate rate-law formulations that reflect finer-scale behavior from empirical considerations, and preparing preliminary constitutive models that can be used as interim input for high-fidelity code design and applications.

The intricacy of the upscaling process, and the requirement to develop VU-assessed methods that propagate uncertainties, mandates a staged approach, where complexity is introduced into the simulation system incrementally, so that each step is individually assessed. From the atomistic scale, the initial development will begin with dissolution of an aluminosilicate mineral

(orthoclase). The atomic composition and dissolution of orthoclase shares some key characteristics with glass, enabling development of needed upscaling methods on a much simpler chemical system. Because orthoclase is a well-characterized, ordered mineral that has been studied in great detail, sufficient high-quality data on its dissolution exist (and additional data can be generated) to support the development and validation of the chemical models. The interim goals are to reproduce observed dissolution rates as a function of the crystal surface orientation, pH, and temperature, and to develop methods of aggregating the chemical processes to obtain effective upscaled rate laws with explicit dependency on pH and temperature. The expectation is that the process of upscaling will be similar for amorphous silicates and other complex compositions, but that the chemical system will be correspondingly more complex.

Additional intermediate steps in the challenge milestone will introduce additional complexity incrementally. These steps include generating models of the amorphous glass surfaces, incorporating the reactivity of the heterogeneous bonding network into effective rate laws, adding chemical constituents (e.g., sodium, boron, aluminum, radionuclides, etc.) that reflect the complex composition of candidate glass waste forms, and modeling the microstructural evolution of the bulk waste form, with a consequent increase in the aqueous-accessible surface and the dissolution rate.

Simultaneously, the continuum rate laws available will be assessed relative to empirical data from glass systems (e.g. corrosion of archeological glass, glass leaching studies), and new rate laws will be developed that incorporate the atomistic level. As more mechanistic rate equations are developed and the understanding of glass dissolution improves, additional targeted atomistic simulations will be conducted to identify, explain, and quantify the phenomena suggested by the development of accurate rate laws for continuum modeling. The improved rate law formulations will serve to identify important sub-continuum phenomena, support FEP evaluation, and provide guidance for prioritization of sub-continuum scale efforts. These preliminary constitutive models will also serve as input for high-fidelity continuum simulations.

The incremental steps in the challenge milestone can and will be concurrently investigated, with the overall upscaling process created as a careful composition of the individual step. Concurrent activities may include defining an upscaling process for orthoclase dissolution, generating and validating glass dissolution models, and simulating amorphous surface chemistry.

Ideally, the ultimate goal of the challenge milestone is to develop a capability for creating constitutive models on-demand for waste form dissolution. This would consist of a systematic methodology starting with a waste glass of a specified composition in a given EBS environment and a description of fundamental chemical process and ending with effective constitutive rate equations using protocols that propagate uncertainties through the upscaling method.

3.2.2. Code Capabilities to be Demonstrated

Upscaling

- Computation of energetics of fundamental chemical processes for glass corrosion and dissolution: reaction energies (quantum chemistry) and diffusion energies (quantum chemistry and classical molecular dynamics)

- Computational aggregation of fundamental chemical processes into effective collective rate laws for glass dissolution
- Simulation of microstructural evolution and compositional changes involved in corrosion and dissolution at glass surfaces (or development of effective empirical proxies)
- Coupled high-fidelity models

High-Fidelity Continuum Code Capabilities

- Continuum simulation of glass dissolution: formulation of effective rate laws with coupled chemical and hydrological properties
- Code capabilities from Challenge Milestone 1
- Chemical reaction with explicit reaction kinetics
- Simulation of waste package corrosion (e.g., general, localized, microbially-induced)
- Accounting for spatial variability in the values for the parameters for each corrosion functional form, where variability can occur among local areas comprising the surface of an individual waste package
- Simulation of waste package stress corrosion cracking
- Simulation of radiolysis effects
- Thermal-hydrological-chemical coupling with explicit reactive transport
- Uncertainty quantification for data transfer from sub-continuum simulations to constitutive models and high-fidelity simulations

Performance Assessment Code Capabilities

The same capabilities will be implemented as for the high-fidelity model, but in an abstracted form or at reduced resolution/dimension. In addition, the PA code will:

- Uncertainty quantification for data transfer from high-fidelity simulations to PA models

3.2.3. V&V Needs

- Develop V&V and UQ protocols for sub-continuum codes and associated calculations
- Methods for propagating uncertainties filtered through upscaling: aware of both form of physics abstraction and in specific realization (populating parameters) of the constitutive models
- Methods for validating resolution of spatial and temporal discretization.
- System for information capture and management, protocols for collecting and storing V&V evidence
- Experimental data on package-scale testing of waste form degradation
- Manufactured solutions for THC coupling

3.2.4. Data Needs

- Validation data for models of dissolution of well-characterized silicate systems: kinetic dissolution rates as a function of environmental conditions (pH and temperature) for orthoclase, a simple amorphous glass, and glasses of controlled composition

- Validation data for models of archeological (or other) glass corrosion: experimental analysis (with chemical gradients from the glass surface through the near-field) and characterization of pristine glass and corrosion layers
- Structure evolution of corroded glass surface with reaction extent and time
- Representative elemental composition and structure of proxies for candidate high-level waste glass materials
- Kinetic data on high level waste glass degradation over the anticipated range of environmental conditions
- Data on waste package corrosion and failure over the anticipated range of environmental conditions
- Thermodynamic data for radionuclide source term calculations over the anticipated range of environmental conditions
- Radionuclide inventory
- Physical configuration and boundary conditions

3.3. Challenge Milestone 3: Tunnel Closure (Salt Creep)

3.3.1. Description

Physical Processes and Couplings

As soon as a tunnel is mined in salt, the hydrostatic state of stress in the salt is disturbed and deviatoric stresses are introduced in the salt. There is also a region, immediately surrounding the excavation, which is disturbed and partially damaged due to the mining of the opening (the excavation disturbed zone, EDZ). As a consequence of the excavation process, the salt begins to creep in response to the deviatoric stresses and this leads to very large deformations of the tunnel opening (roof/ribs/floor) and eventually to a complete closure of the tunnel and encapsulation of the waste. In addition to the creep of the salt induced by the deviatoric stresses at ambient conditions, creep of salt is also highly dependent on temperature. The creep rate will be accelerated beyond that at ambient conditions due to the thermal load generated once the high-level waste is emplaced and begins to heat the salt. The conceptual model for this challenge milestone includes backfill (crushed salt) emplaced around the waste packages that would inhibit creep of the surrounding salt formation and provide shielding protection to allow for continued emplacement of other waste packages in adjacent openings. The degradation of the waste packages could potentially lead to generation of gas in the tunnel, which could further inhibit tunnel closure due to salt creep to some degree. Consequently, the capability to model the coupled thermal-hydrological-mechanical (THM) processes that result in tunnel deformation/closure due to the presence of a thermal field and/or pressure gradients that evolve with time is needed. This milestone focuses on the tunnel deformation/closure due to salt creep and the movement of moisture along with the deforming salt (i.e., in intercrystalline porosity or fluid inclusions). Challenge Milestone 4 (Section 3.4) focuses on the movement of moisture within the EBS (i.e., through the tunnel openings, through the pore space in the backfill, and around the waste forms and waste packages).

Model Implementation

Both the high-fidelity and the PA models will calculate the large deformations and closure of the tunnel and the thermal transfer in the tunnel and surrounding rock as a function of water content

in the various materials, the geologic stratigraphy, boundary conditions, any potential gas generation, and the physical configuration of the waste packages.

High-Fidelity Continuum Model: In the high-fidelity model, the tunnel and a representative extent of material (including other geologic strata) above and below the excavation, any backfill, and a representation of the waste packages will be modeled with a 3-D high resolution mesh to capture the heterogeneity of the materials in the tunnel and surrounding rock. The high fidelity model will be intended to capture detailed spatial and temporal evolution of deformation and thermal transfer in the tunnel.

Performance Assessment Model: In the PA model, the tunnel closure will be implemented with a simplified, reduced-resolution representation based on the high-fidelity continuum model. The PA model will also focus on uncertainty quantification through input parameter sampling and multiple model calculations.

3.3.2. Code Capabilities to be Demonstrated

High-Fidelity Continuum Code Capabilities

- Simulation of temperature dependent, quasi-static, large-deformation solid mechanics in geologic media
- Simulation of contact interaction mechanics at interfaces (in stratigraphy and various surfaces of tunnel) and heat transfer across interfaces
- Simulation of fluid movement along with deforming geologic media
- Provide constitutive relationships for elevated temperature creep of salt and for elevated temperature-dependent response of appropriate non-salt materials
- Simulation of heat transport in non-isothermal systems by convection, conduction, and radiant heat transfer

Performance Assessment Code Capabilities

The same capabilities will be implemented as for the high-fidelity model, but in an abstracted form or at reduced resolution/dimension. In addition, the PA code will:

- Sample input parameter distributions and uncertainty propagation

3.3.3. V&V Needs

High-Fidelity Continuum Code Verification

- Test cases for simulating temperature dependent, quasi-static, large-deformation solid mechanics in geologic media (e.g., those used for WIPP at lower temperatures)
- Test cases for simulating contact interaction mechanics at interfaces
- Test cases for simulating fluid movement along with deforming geologic media
- Test cases for simulating heat transport in non-isothermal systems by convection, conduction, and radiant heat transfer
- Test cases for 1-, 2- and 3-dimensional flow and transport problems
- Methods for validating resolution of spatial and temporal discretization.
- Test cases for demonstrating evaporation/condensation-flux simulation

Performance Assessment Code Verification

- Test cases for demonstrating the ability of the PA model to mimic the high fidelity model functionalities and results
- Test cases demonstrating sampling input parameter distribution and uncertainty propagation functionalities

Model Validation

- Experimental data, (e.g., for room (tunnel) closure measurements from WIPP or other salt repositories)

3.3.4. Data Needs

- Stratigraphy above and below tunnel, representative of a generic salt formation
- Mechanical properties of various materials in tunnel and surrounding stratigraphy
- Water content in various materials in tunnel and surrounding stratigraphy
- Thermal properties in tunnel and surrounding stratigraphy
- Physical configuration and boundary conditions
- Field-scale measurements of salt creep and moisture movement within the salt (i.e., in intercrystalline porosity or fluid inclusions)
- Measurements of salt creep in the presence of a backstress (e.g., gas pressure, waste package)

3.4. Challenge Milestone 4: Heat and Fluid Movement in the Near Field

3.4.1. Description

Physical Processes and Couplings

Within the EBS, the backfill will contain some amount of natural moisture. There will also be some water (brine) in the near-field host rock salt formation and in other geologic strata that may intersect the salt formation. Fluid in the EBS may experience a complex set of phase transitions including evaporation, boiling, and condensation. The various fluid phases within the EBS may also evolve as the thermal load generated from the waste evolves with time. The presence of moisture in the EBS in the immediate vicinity of the waste form and waste packages can lead to degradation (see Challenge Milestone 2 in Section 3.2). Waste form and waste package degradation are also temperature dependent, as is water chemistry (See Challenge Milestone 1, Section 3.1), which is the driver for degradation. Consequently, the capability to model the coupled thermal-hydrological-chemical (THC) processes that result in movement of heat and fluid within the EBS (i.e., around the waste forms and waste packages and within the tunnel openings and pore space within the salt backfill) due to the presence of a thermal field and/or pressure gradients that evolve with time is needed. In Challenge Milestone 5 (Section 3.5), the THC capabilities developed in this milestone will be coupled with the THM capabilities developed in Challenge Milestone 3 (Section 3.3), to produce a complete treatment of the coupled THCM effects of heat and fluid movement in the near field of a disposal system located in a salt formation.

Model Implementation

Both the high-fidelity and the PA models will calculate heat and fluid movement in the EBS as a function of water chemistry, degradation kinetics of waste form and waste package materials and any accompanying gas generation, and the physical configuration of the waste packages.

High-Fidelity Continuum Model: In the high-fidelity model, the EBS (potentially including the excavation disturbed zone) and a representation of the waste packages will be modeled with a 3-D high resolution mesh to capture the heterogeneity of the materials in the EBS (including any air gap). The high-fidelity model will be intended to capture detailed spatial and temporal evolution of heat and fluid flow within the EBS.

Performance Assessment Model: In the PA model, the EBS components will be treated as coarsely gridded compartments derived from the high-fidelity continuum model representation. The PA model will be focused on uncertainty quantification through input parameter sampling and simulation of multiple realizations.

3.4.2. Code Capabilities to be Demonstrated

High-Fidelity Continuum Code Capabilities

- Calculation of flow processes including pressure-driven gas flow, pressure driven liquid flow, gravity effects, capillary effects, and viscous force effects on flows
- Simulation of flow processes in the backfill, tunnel openings, and near-field host rock
- Provide constitutive relationships for vapor-pressure lowering, and temperature-dependent capillary pressure
- Simulation of multiphase fluid flow, and multi-component flow and chemical reactions
- Simulation of phase changes and binary diffusion in the gas phase
- Simulation of heat transport in non-isothermal systems by convection, conduction, radiant heat transfer, and coupled fluid and heat flow
- Simulation of reaction of the fluids (aqueous solutions and gases) with the solids in the coupled thermal-hydrologic system
- Solution of 1-, 2- and 3-dimensional flow problems

Performance Assessment Code Capabilities

The same capabilities will be implemented as for the high-fidelity model, but in an abstracted form or at reduced resolution/dimension. In addition, the PA code will:

- Sample input parameter distributions

3.4.3. V&V Needs

High-Fidelity Continuum Code Verification

- Test cases for calculating flow processes including pressure-driven gas flow, pressure driven liquid flow, gravity effects, capillary effects, and viscous force effects on flows
- Test cases for simulating flow processes in porous media and tunnel openings
- Test cases for demonstrating constitutive relationships for vapor-pressure lowering, and temperature-dependent capillary pressure

- Test cases for simulating multiphase fluid flow, and multi-component flow, coupled chemical reactions, and transport
- Test cases for simulating phase changes and binary diffusion in the gas phase
- Test cases for simulating heat transport in non-isothermal systems by convection, conduction, radiant heat transfer, and coupled fluid and heat flow
- Test cases for simulating reaction of the fluids (aqueous solutions and gases) with the solids in the system in a coupled manner with the thermal-hydrologic system
- Test cases for solving 1-, 2- and 3-dimensional flow problems
- Methods for validating resolution of spatial and temporal discretization.
- Manufactured solutions for THM coupling

Performance Assessment Code Verification

- Test cases for demonstrating the ability of the PA model to mimic the high fidelity model functionalities and results
- Test cases for demonstrating the ability to sample input parameter distributions and uncertainty propagation

Model Validation

- Experimental data

3.4.4. Data Needs

- Physical configuration and boundary conditions
- Fluid and material properties governing heat and fluid flow
- Water content in various materials in tunnel and surrounding stratigraphy
- Thermal properties in tunnel and surrounding stratigraphy
- Tunnel-scale measurements of heat and moisture movement

3.5. Challenge Milestone 5: Radionuclide Mobilization and Transport in the Near Field

3.5.1. Description

Physical Processes and Couplings

This milestone will integrate the capabilities from the previous four milestones and add radionuclide transport capabilities to produce a coupled THCM model. The degradation of waste packages and HLW borosilicate glass waste forms emplaced within a salt repository (salt backfill within a salt host rock formation), will lead to the mobilization and transport of radionuclides through pathways in the EBS, the adjacent EDZ, and the host rock. The heat load from the waste will influence fluid movement and radionuclide transport and tunnel deformation/closure due to salt creep will alter the transport pathways. The presence of moisture may also enhance degradation of the waste packages and potentially lead to generation of gas in the tunnel, which could inhibit tunnel closure due to salt creep to some degree. This milestone will develop the capability to couple these thermal-hydrological-chemical-mechanical (THCM) processes and simulate the aqueous-phase transport of dissolved radionuclides in the near field of a deforming

salt repository. Radionuclide transport capabilities may be expanded to include gas-phase transport and/or colloid-associated radionuclides.

Model Implementation

High-Fidelity Continuum Model: In the high-fidelity model, the tunnel and a representative extent of material surrounding the tunnel, the salt backfill, and a representation of the waste forms and waste packages will be modeled with a 3-D high resolution mesh to capture the heterogeneity of the materials in the tunnel and surrounding rock. Three-dimensional multiphase flow and transport simulations will be performed with high spatial resolution, sufficient to capture the individual waste packages. The high-fidelity model will be intended to capture detailed spatial and temporal evolution of deformation, heat and fluid movement, chemical reactions, and radionuclide transport occurring in the near field.

Performance Assessment Model: In the PA model, the EBS will be represented by a set of coarsely divided compartments, and waste packages will be grouped according to their failure modes and breach times. The representation of the coupled THCM processes governing deformation, heat and fluid movement, chemical reactions, and radionuclide transport will be informed by the high-fidelity model simulations. The PA model will be focused on quantifying the uncertainty for the data transfer from the high-fidelity model to the PA model.

3.5.2. Code Capabilities to be Demonstrated

High-Fidelity Continuum Code Capabilities

- Integration of code capabilities from Challenge Milestones 1 through 4
- Accounting for spatial variability in the values for the parameters for each corrosion functional form, where variability can occur from waste package to waste package
- Multi-component geochemical computations accounting for both reversible and irreversible chemical processes
- Solution of 1-, 2- and 3-dimensional multi-phase fluid flow and radionuclide transport problems
- Simulation of radioactive decay and ingrowth
- Coupled THCM model for salt creep and moisture movement in the presence of thermal and/or pressure gradients

Performance Assessment Code Capabilities

The same capabilities will be implemented as for the high-fidelity model, but in an abstracted form or at reduced resolution/dimension. In addition, the PA code will:

- Sample input parameter distributions
- Provide capabilities for inputs and outputs of multiple realizations

3.5.3. V&V Needs

High-Fidelity Continuum Code Verification

- Relevant test cases from Challenge Milestones 1 through 4, applied to the coupled model
- Test cases for simulating multi-component geochemical computations based on chemical mass-action and mass balance

- Test cases for computing the starting concentration of any primary species, assuming equilibrium with a mineral or gas at a given fugacity
- Test cases demonstrating the capability of allowing charge balance of an input solution to be achieved by adjusting the concentration of a given primary species
- Test cases for solving 1-, 2- and 3-dimensional multi-phase fluid flow and radionuclide transport problems
- Test cases demonstrating radioactive decay and ingrowth
- Methods for validating resolution of spatial and temporal discretization.
- Manufactured solutions for THCM coupling

Performance Assessment Code Verification

- Test cases for demonstrating the ability of the PA model to mimic the high fidelity model functionalities and results
- Test cases demonstrating sampling input parameter distributions

Model Validation

- Experimental data
- Independent technical/peer review

3.5.4. Data Needs

- Integration of data from Challenge Milestones 1 through 4
- Properties of the fluids and EBS materials controlling radionuclide transport
- Chemical kinetics related to radionuclide transport
- Tunnel-scale THCM testing data

4. SUMMARY

This report describes the specification of a challenge problem for the NEAMS Waste IPSC. The Waste IPSC challenge problem includes coupled THCM processes that describe (1) the degradation of a borosilicate glass waste form and the corresponding mobilization of radionuclides (i.e., the processes that produce the radionuclide source term), (2) the associated near-field physical and chemical environment for waste emplacement within a salt formation, and (3) radionuclide transport in the near field (i.e., through the engineered components – waste form, waste package, and backfill - and the immediately adjacent salt). A set of milestones that collectively comprise the full challenge problem are also specified.

The overarching Waste IPSC goal is to develop an integrated suite of modeling and simulation capabilities to simulate the long-term performance of waste forms in the engineered and geologic environments of a radioactive waste storage or disposal system for a range of disposal concepts, waste form types, engineered repository designs, and geologic settings. The Waste IPSC challenge problem milestones demonstrate proof of concept and progress towards the overarching Waste IPSC goal.

The Waste IPSC challenge problem and associated milestones require the development of (1) constitutive relationships derived from sub-continuum processes, (2) coupled (physically and numerically) THCMBR process models, and (3) advanced (VU-assessed) V&V and UQ approaches, where possible. The development and implementation of these advanced modeling and simulation capabilities will represent a significant advancement in applicability, representation of fundamental principles, THCM coupling, and technical defensibility over currently available codes.

The Waste IPSC challenge problem satisfies the NEAMS challenge problem criteria (see Section 1.1). The challenge problem (1) supports DOE-NE Research and Development Objective 3 (Develop Sustainable Nuclear Fuel Cycles) by providing a tool to evaluate and inform radioactive waste disposal, a key aspect of any fuel cycle; (2) is a problem of interest to numerous stakeholders, including the DOE-NE WF and UFD Campaigns, the BRC, and NRC; (3) breaks new technical ground through the development and application of advanced modeling and simulation techniques to describe the coupled multi-physics that are representative of a disposal system; (4) is computationally demanding and scientifically complex; and (5) provides milestones against which progress and success can be measured.

5. REFERENCES

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APPENDIX A: FEATURES, EVENTS, AND PROCESSES (FEPS) POTENTIALLY RELEVANT TO THE WASTE IPSC

A preliminary set of 208 FEPs potentially relevant to the technical scope and range of disposal system alternatives that need to be evaluated and/or implemented within the Waste IPSC are listed in Table A-1. As described in Section 2.1.1, these FEPs were developed from existing FEP lists and other relevant information (NEA 1999 Appendix D; NEA 2006; SNL 2008, Table 7-1; SNL 2009, Section 3). The FEPs are organized using a hierarchical numbering system that groups similar FEPs together.

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC

UFD FEP Number	Description	Associated Processes	Challenge Milestone
0.0.00.00	0. ASSESSMENT BASIS		
0.1.02.01	Timescales of Concern		All
0.1.03.01	Spatial Domain of Concern		All
0.1.09.01	Regulatory Requirements and Exclusions		N/A
0.1.10.01	Model Issues	<ul style="list-style-type: none"> - Conceptual model - Mathematical implementation - Geometry and dimensionality - Process coupling - Boundary and initial conditions 	All
0.1.10.02	Data Issues	<ul style="list-style-type: none"> - Parameterization and values - Correlations - Uncertainty 	All
1.0.00.00	1. EXTERNAL FACTORS		
1.1.00.00	1. REPOSITORY ISSUES		
1.1.01.01	Open Boreholes	<ul style="list-style-type: none"> - Site investigation boreholes (open, improperly sealed) - Preclosure and postclosure monitoring boreholes - Enhanced flow pathways from EBS 	3,4
1.1.02.01	Chemical Effects from Preclosure Operations <ul style="list-style-type: none"> - In EBS - In EDZ - In Host Rock 	<ul style="list-style-type: none"> - Water contaminants (explosives residue, diesel, organics, etc.) - Water chemistry different than host rock (e.g., oxidizing) - Undesirable materials left - Accidents and unplanned events 	1,2,5
1.1.02.02	Mechanical Effects from Preclosure Operations <ul style="list-style-type: none"> - In EBS - In EDZ - In Host Rock 	<ul style="list-style-type: none"> - Creation of excavation-disturbed zone (EDZ) - Stress relief - Boring and blasting effects - Rock reinforcement effects (drillholes) - Accidents and unplanned events - Enhanced flow pathways <p>[see also Evolution of EDZ in 2.2.01.01]</p>	3,4,5
1.1.02.03	Thermal-Hydrologic Effects from Preclosure Operations <ul style="list-style-type: none"> - In EBS - In EDZ - In Host Rock 	<ul style="list-style-type: none"> - Site flooding - Preclosure ventilation - Accidents and unplanned events 	3,4,5

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
1.1.08.01	Deviations from Design and Inadequate Quality Control	<ul style="list-style-type: none"> - Error in waste emplacement (waste forms, waste packages, waste package support materials) - Error in EBS component emplacement (backfill, seals, liner) - Inadequate excavation / construction (planning, schedule, implementation) - Aborted / incomplete closure of repository - Material and/or component defects 	N/A
1.1.10.01	Control of Repository Site	<ul style="list-style-type: none"> - Active controls (controlled area) - Retention of records - Passive controls (markers) 	N/A
1.1.13.01	Retrievability		N/A
1.2.00.00	2. GEOLOGICAL PROCESSES AND EFFECTS		
1.2.01.00	2.01. LONG-TERM PROCESSES		
1.2.01.01	Tectonic Activity – Large Scale	<ul style="list-style-type: none"> - Uplift - Folding 	N/A
1.2.02.01	Subsidence		3
1.2.05.01	Metamorphism	<ul style="list-style-type: none"> - Structural changes due to natural heating and/or pressure 	N/A
1.2.08.01	Diagenesis	<ul style="list-style-type: none"> - Mineral alteration due to natural processes 	N/A
1.2.09.01	Diapirism	<ul style="list-style-type: none"> - Plastic flow of rocks under lithostatic loading - Salt / evaporates - Clay 	N/A
1.2.09.02	Large-Scale Dissolution		N/A
1.2.03.00	2.03. SEISMIC ACTIVITY		
1.2.03.01	Seismic Activity Impacts EBS and/or EBS Components	<ul style="list-style-type: none"> - Mechanical damage to EBS (from ground motion, rockfall, drift collapse, fault displacement) <p>[see also Mechanical Impacts in 2.1.07.04, 2.1.07.05, 2.1.07.06, 2.1.07.07, 2.1.07.08, and 2.1.07.10]</p>	3,5
1.2.03.02	Seismic Activity Impacts Geosphere - Host Rock - Other Geologic Units	<ul style="list-style-type: none"> - Altered flow pathways and properties - Altered stress regimes (faults, fractures) <p>[see also Alterations and Impacts in 2.2.05.01, 2.2.05.02, 2.2.05.03, 2.1.07.01, and 2.1.07.02]</p>	N/A
1.2.03.03	Seismic Activity Impacts Biosphere - Surface Environment - Human Behavior	<ul style="list-style-type: none"> - Altered surface characteristics - Altered surface transport pathways - Altered recharge 	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
1.2.04.00	2.04. IGNEOUS ACTIVITY		
1.2.04.01	Igneous Activity Impacts EBS and/or EBS Components	<ul style="list-style-type: none"> - Mechanical damage to EBS (from igneous intrusion) - Chemical interaction with magmatic volatiles - Transport of radionuclides (in magma, pyroclasts, vents) <p>[see also Mechanical Impacts in 2.1.07.04, 2.1.07.05, 2.1.07.06, 2.1.07.07, and 2.1.07.08]</p>	3,5
1.2.04.02	Igneous Activity Impacts Geosphere - Host Rock - Other Geologic Units	<ul style="list-style-type: none"> - Altered flow pathways and properties - Altered stress regimes (faults, fractures) - Igneous intrusions - Altered thermal and chemical conditions <p>[see also Alterations and Impacts in 2.2.05.01, 2.2.05.02, 2.2.05.03, 2.1.07.01, 2.1.07.02, 2.2.09.03, 2.2.11.06 and 2.2.11.07]</p>	N/A
1.2.04.03	Igneous Activity Impacts Biosphere - Surface Environment - Human Behavior	<ul style="list-style-type: none"> - Altered surface characteristics - Altered surface transport pathways - Altered recharge - Ashfall and ash redistribution 	N/A
1.3.00.00	3. CLIMATIC PROCESSES AND EFFECTS		
1.3.01.01	Climate Change - Natural - Anthropogenic	<ul style="list-style-type: none"> - Variations in precipitation and temperature - Long-term global (sea level, ...) - Short-term regional and local - Seasonal local (flooding, storms, ...) <p>[see also Human Influences on Climate in 1.4.01.01] [contributes to Precipitation in 2.3.08.01, Surface Runoff and Evapotranspiration in 2.3.08.02]</p>	N/A
1.3.04.01	Periglacial Effects	<ul style="list-style-type: none"> - Permafrost - Seasonal freeze/thaw 	N/A
1.3.05.01	Glacial and Ice Sheet Effects	<ul style="list-style-type: none"> - Glaciation - Isostatic depression - Melt water 	N/A
1.4.00.00	4. FUTURE HUMAN ACTIONS		
1.4.01.01	Human Influences on Climate - Intentional - Accidental	<ul style="list-style-type: none"> - Variations in precipitation and temperature - Global, regional, and/or local - Greenhouse gases, ozone layer failure <p>[contributes to Climate Change in 1.3.01.01]</p>	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
1.4.02.01	Human Intrusion - Deliberate - Inadvertent	- Drilling (resource exploration, ...) - Mining / tunneling - Unintrusive site investigation (airborne, surface-based, ...) [see also Control of Repository Site in 1.1.10.01]	5
1.4.11.01	Explosions and Crashes from Human Activities	- War - Sabotage - Testing - Resource exploration / exploitation - Aircraft	N/A
1.5.00.00	5. OTHER		
1.5.01.01	Meteorite Impact	- Cratering, host rock removal - Exhumation of waste - Alteration of flow pathways	N/A
1.5.01.02	Extraterrestrial Events	- Solar systems (supernova) - Celestial activity (sun - solar flares, gamma-ray bursters; moon – earth tides) - Alien life forms	N/A
1.5.03.01	Earth Planetary Changes	- Changes in earth's magnetic field - Changes in earth's gravitational field (tides)	N/A
2.0.00.00	2. DISPOSAL SYSTEM FACTORS		
2.1.00.00	1. WASTES AND ENGINEERED FEATURES		
2.1.01.00	1.01. INVENTORY		
2.1.01.01	Waste Inventory - Radionuclides - Non-Radionuclides	- Composition - Enrichment / Burn-up	1,2,5
2.1.01.02	Radioactive Decay and Ingrowth		1,2,5
2.1.01.03	Heterogeneity of Waste Inventory - Waste Package Scale - Repository Scale	- Composition - Enrichment / Burn-up - Damaged Area	1,2,5
2.1.01.04	Interactions Between Co-Located Waste		1,2,5

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.02.00	1.02. WASTE FORM		
2.1.02.01	SNF (Commercial, DOE) Degradation - Alteration / Phase Separation - Dissolution / Leaching - Radionuclide Release	Degradation is dependent on: - Composition - Geometry / Structure - Enrichment / Burn-up - Surface Area - Gap and Grain Fraction - Damaged Area - THC Conditions [see also Mechanical Impact in 2.1.07.06 and Thermal-Mechanical Effects in 2.1.11.06]	1,2
2.1.02.02	HLW (Glass, Ceramic, Metal) Degradation - Alteration / Phase Separation - Dissolution / Leaching - Cracking - Radionuclide Release	Degradation is dependent on: - Composition - Geometry / Structure - Surface Area - Damaged / Cracked Area - Mechanical Impact - THC Conditions [see also Mechanical Impact in 2.1.07.07 and Thermal-Mechanical Effects in 2.1.11.06]	1,2
2.1.02.03	Degradation of Organic/Cellulosic Materials in Waste	[see also Complexation in EBS in 2.1.09.54]	1,2
2.1.02.04	HLW (Glass, Ceramic, Metal) Recrystallization		2
2.1.02.05	Pyrophoricity or Flammable Gas from SNF or HLW	[see also Gas Explosions in EBS in 2.1.12.04]	2
2.1.02.06	SNF Cladding Degradation and Failure	- Initial damage - General Corrosion - Microbially Influenced Corrosion - Localized Corrosion - Enhanced Corrosion (silica, fluoride) - Stress Corrosion Cracking - Hydride Cracking - Unzipping - Creep - Internal Pressure - Mechanical Impact	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.03.00	1.03. WASTE CONTAINER		
2.1.03.01	Early Failure of Waste Packages	- Manufacturing defects - Improper sealing [see also Deviations from Design in 1.1.08.01]	2
2.1.03.02	General Corrosion of Waste Packages	- Dry-air oxidation - Humid-air corrosion - Aqueous phase corrosion - Passive film formation and stability	2
2.1.03.03	Stress Corrosion Cracking (SCC) of Waste Packages	- Crack initiation, growth and propagation - Stress distribution around cracks	2
2.1.03.04	Localized Corrosion of Waste Packages	- Pitting - Crevice corrosion - Salt deliquescence [see also 2.1.09.06 Chemical Interaction with Backfill]	2
2.1.03.05	Hydride Cracking of Waste Packages	- Hydrogen diffusion through metal matrix - Crack initiation and growth in metal hydride phases	2
2.1.03.06	Microbially Influenced Corrosion (MIC) of Waste Packages		2
2.1.03.07	Internal Corrosion of Waste Packages Prior to Breach		2
2.1.03.08	Evolution of Flow Pathways in Waste Packages	- Evolution of physical form of waste package - Plugging of cracks in waste packages [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Mechanical Impacts in 2.1.07.05, 2.1.07.06, and 2.1.07.07, Thermal-Mechanical Effects in 2.1.11.06 and 2.1.11.07]	3,4
2.1.04.00	1.04. BUFFER / BACKFILL		
2.1.04.01	Evolution and Degradation of Backfill	- Alteration - Thermal expansion / Degradation - Swelling / Compaction - Erosion / Dissolution - Evolution of backfill flow pathways [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Mechanical Impact in 2.1.07.04, Thermal-Mechanical Effects in 2.1.11.08, Chemical Interaction in 2.1.09.06]	3,4,5
2.1.05.00	1.05. SEALS		
2.1.05.01	Degradation of Seals	- Alteration / Degradation / Cracking - Erosion / Dissolution [see also Mechanical Impact in 2.1.07.08, Thermal-Mechanical Effects in 2.1.11.09, Chemical Interaction in 2.1.09.08]	3,4,5

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.06.00	1.06. OTHER EBS MATERIALS		
2.1.06.01	Degradation of Liner / Rock Reinforcement Materials in EBS	<ul style="list-style-type: none"> - Alteration / Degradation / Cracking - Corrosion - Erosion / Dissolution / Spalling <p>[see also Mechanical Impact in 2.1.07.08, Thermal-Mechanical Effects in 2.1.11.09, Chemical Interaction in 2.1.09.07]</p>	3,4,5
2.1.07.00	1.07. MECHANICAL PROCESSES		
2.1.07.01	Rockfall	<ul style="list-style-type: none"> - Dynamic loading (block size and velocity) <p>[see also Mechanical Effects on Host Rock in 2.2.07.01]</p>	3
2.1.07.02	Drift Collapse	<ul style="list-style-type: none"> - Static loading (rubble volume) - Alteration of seepage - Alteration of EBS flow pathways - Alteration of EBS thermal environment <p>[see also Evolution of Flow Pathways in EBS in 2.1.08.06, Chemical Effects of Drift Collapse in 2.1.09.12, and Effects of Drift Collapse on TH in 2.1.11.04, Mechanical Effects on Host Rock in 2.2.07.01]</p>	3,4
2.1.07.03	Mechanical Effects of Backfill	<ul style="list-style-type: none"> - Protection of other EBS components from rockfall / drift collapse 	3,4
2.1.07.04	Mechanical Impact on Backfill	<ul style="list-style-type: none"> - Rockfall / Drift collapse - Hydrostatic pressure - Internal gas pressure <p>[see also Degradation of Backfill in 2.1.04.01 and Thermal-Mechanical Effects in 2.1.11.08]</p>	3
2.1.07.05	Mechanical Impact on Waste Packages	<ul style="list-style-type: none"> - Rockfall / Drift collapse - Waste package movement - Hydrostatic pressure - Internal gas pressure - Swelling corrosion products <p>[see also Thermal-Mechanical Effects in 2.1.11.07]</p>	3
2.1.07.06	Mechanical Impact on SNF Waste Form	<ul style="list-style-type: none"> - Drift collapse - Swelling corrosion products <p>[see also Thermal-Mechanical Effects in 2.1.11.06]</p>	3
2.1.07.07	Mechanical Impact on HLW Waste Form	<ul style="list-style-type: none"> - Drift collapse - Swelling corrosion products <p>[see also Thermal-Mechanical Effects in 2.1.11.06]</p>	3

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.07.08	Mechanical Impact on Other EBS Components - Seals - Liner/Rock Reinforcement Materials - Waste Package Support Materials	- Rockfall / Drift collapse - Movement - Hydrostatic pressure - Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.09]	3
2.1.07.09	Mechanical Effects at EBS Component Interfaces	- Component-to-component contact (static or dynamic)	3
2.1.07.10	Mechanical Degradation of EBS	- Floor buckling - Fault displacement - Initial damage from excavation / construction - Consolidation of EBS components - Degradation of waste package support structure - Alteration of EBS flow pathways [see also Mechanical Effects from Preclosure in 1.1.02.02, Evolution of Flow Pathways in EBS in 2.1.08.06, Drift Collapse in 2.1.07.02, Degradation in 2.1.04.01, 2.1.05.01, and 2.1.06.01, and Mechanical Effects on Host Rock in 2.2.07.01]	3,4,5
2.1.08.00	1.08. HYDROLOGIC PROCESSES		
2.1.08.01	Flow Through the EBS	- Saturated / Unsaturated flow - Preferential flow pathways - Density effects on flow - Initial hydrologic conditions - Flow pathways out of EBS [see also Open Boreholes in 1.1.01.01, Thermal-Hydrologic Effects from Preclosure in 1.1.02.03, Flow in Waste Packages in 2.1.08.02, Flow in Backfill in 2.1.08.03, Flow through Seals 2.1.08.04, Flow through Liner in 2.1.08.05, Thermal Effects on Flow in 2.1.11.10, Effects of Gas on Flow in 2.1.12.02]	4
2.1.08.02	Flow In and Through Waste Packages	- Saturated / Unsaturated flow - Movement as thin films or droplets	2,4
2.1.08.03	Flow in Backfill	- Fracture / Matrix flow	4
2.1.08.04	Flow Through Seals		4
2.1.08.05	Flow Through Liner / Rock Reinforcement Materials in EBS		4

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.08.06	Alteration and Evolution of EBS Flow Pathways	<ul style="list-style-type: none"> - Drift collapse - Degradation/consolidation of EBS components - Plugging of flow pathways - Formation of corrosion products - Water ponding <p>[see also Evolution of Flow Pathways in WPs in 2.1.03.08, Evolution of Backfill in 2.1.04.01, Drift Collapse in 2.1.07.02, and Mechanical Degradation of EBS in 2.1.07.10]</p>	3,4,5
2.1.08.07	Condensation Forms in Repository - On Tunnel Roof / Walls - On EBS Components	<ul style="list-style-type: none"> - Heat transfer (spatial and temporal distribution of temperature and relative humidity) - Dripping <p>[see also Heat Generation in EBS in 2.1.11.01, Effects on EBS Thermal Environment in 2.1.11.03 and 2.1.11.04]</p>	4
2.1.08.08	Capillary Effects in EBS	<ul style="list-style-type: none"> - Wicking 	4
2.1.08.09	Influx/Seepage Into the EBS	<ul style="list-style-type: none"> - Water influx rate (spatial and temporal distribution) <p>[see also Open Boreholes in 1.1.01.01, Thermal Effects on Flow in EBS in 2.1.11.10, Flow Through Host Rock in 2.2.08.01, Effects of Excavation on Flow in 2.2.08.04]</p>	4
2.1.09.00	1.09. CHEMICAL PROCESSES - CHEMISTRY		
2.1.09.01	Chemistry of Water Flowing into the Repository	<ul style="list-style-type: none"> - Chemistry of influent water (spatial and temporal distribution) <p>[See also Chemistry in Host Rock 2.2.09.01]</p>	1,2,5
2.1.09.02	Chemical Characteristics of Water in Waste Packages	<ul style="list-style-type: none"> - Water composition (radionuclides, dissolved species, ...) - Initial void chemistry (air / gas) - Water chemistry (pH, ionic strength, pCO₂, ..) - Reduction-oxidation potential - Reaction kinetics - Influent chemistry (from tunnels and/or backfill) <p>[see also Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]</p> <ul style="list-style-type: none"> - Evolution of water chemistry / interaction with waste packages 	1,2,5

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.09.03	Chemical Characteristics of Water in Backfill	<ul style="list-style-type: none"> - Water composition (radionuclides, dissolved species, ...) - Water chemistry (pH, ionic strength, pCO₂, ..) - Reduction-oxidation potential - Reaction kinetics - Influent chemistry (from tunnels and/or waste package) <p>[see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Tunnels in 2.1.09.04]</p> <ul style="list-style-type: none"> - Evolution of water chemistry / interaction with backfill 	4,5
2.1.09.04	Chemical Characteristics of Water in Tunnels	<ul style="list-style-type: none"> - Water composition (radionuclides, dissolved species, ...) - Water chemistry (pH, ionic strength, pCO₂, ..) - Reduction-oxidation potential - Reaction kinetics - Influent chemistry (from near-field host rock) - Initial chemistry (from construction / emplacement) <p>[see also Chemical Effects from Preclosure in 1.1.02.01, Chemistry of Water Flowing in 2.1.09.01, Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03]</p> <ul style="list-style-type: none"> - Evolution of water chemistry / interaction with seals, liner/rock reinforcement materials, waste package support materials 	4,5
2.1.09.05	Chemical Interaction of Water with Corrosion Products - In Waste Packages - In Backfill - In Tunnels	<ul style="list-style-type: none"> - Corrosion product formation and composition (waste form, waste package internals, waste package) - Evolution of water chemistry in waste packages, in backfill, and in tunnels <p>[contributes to Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]</p>	1,2,5
2.1.09.06	Chemical Interaction of Water with Backfill - On Waste Packages - In Backfill - In Tunnels	<ul style="list-style-type: none"> - Backfill composition and evolution (bentonite, crushed rock, ...) - Evolution of water chemistry in backfill, and in tunnels - Enhanced degradation of waste packages (crevice formation) <p>[contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04, Localized Corrosion of WPs in 2.1.03.04]</p>	1,5

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.09.07	Chemical Interaction of Water with Liner / Rock Reinforcement and Cementitious Materials in EBS - In Backfill - In Tunnels	- Liner composition and evolution (concrete, metal, ...) - Rock reinforcement material composition and evolution (grout, rock bolts, mesh, ...) - Other cementitious materials composition and evolution - Evolution of water chemistry in backfill, and in tunnels [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	1,5
2.1.09.08	Chemical Interaction of Water with Other EBS Components - In Waste Packages - In Tunnels	- Seals composition and evolution - Waste Package Support composition and evolution (concrete, metal, ...) - Other EBS components (other metals (copper), ...) - Evolution of water chemistry in backfill, and in tunnels [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	1,2,5
2.1.09.09	Chemical Effects at EBS Component Interfaces	- Component-to-component contact (chemical reactions) - Consolidation of EBS components	2,5
2.1.09.10	Chemical Effects of Waste-Rock Contact	- Waste-to-host rock contact (chemical reactions) - Component-to-host rock contact (chemical reactions)	2
2.1.09.11	Electrochemical Effects in EBS	- Enhanced metal corrosion	2
2.1.09.12	Chemical Effects of Drift Collapse	- Evolution of water chemistry in backfill and in tunnels (from altered seepage, from altered thermal-hydrology) [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	3,4,5
2.1.09.13	Radionuclide Speciation and Solubility in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	- Dissolved concentration limits - Limited dissolution due to inclusion in secondary phase - Enhanced dissolution due to alpha recoil [controlled by Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	1,2,5
2.1.09.50	1.09. CHEMICAL PROCESSES - TRANSPORT		
2.1.09.51	Advection of Dissolved Radionuclides in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	- Flow pathways and velocity - Advective properties (porosity, tortuosity) - Dispersion - Saturation [see also Gas Phase Transport in 2.1.12.03]	5

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.09.52	Diffusion of Dissolved Radionuclides in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	- Gradients (concentration, chemical potential) - Diffusive properties (diffusion coefficients) - Flow pathways and velocity - Saturation	5
2.1.09.53	Sorption of Dissolved Radionuclides in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	- Surface complexation properties - Flow pathways and velocity - Saturation [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	5
2.1.09.54	Complexation in EBS	- Formation of organic complexants (humates, fulvates, organic waste) - Enhanced transport of radionuclides associated with organic complexants [see also Degradation of Organics in Waste in 2.1.02.03]	5
2.1.09.55	Formation of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	- Formation of intrinsic colloids - Formation of pseudo colloids (host rock fragments, waste form fragments, corrosion products, microbes) - Formation of co-precipitated colloids - Sorption/attachment of radionuclides to colloids (clay, silica, waste form, FeOx, microbes)	2,5
2.1.09.56	Stability of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	- Chemical stability of attachment (dependent on water chemistry) - Mechanical stability of colloid (dependent on colloid size, gravitational settling)	2,5
2.1.09.57	Advection of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	- Flow pathways and velocity - Advective properties (porosity, tortuosity) - Dispersion - Saturation - Colloid concentration	2,5
2.1.09.58	Diffusion of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	- Gradients (concentration, chemical potential) - Diffusive properties (diffusion coefficients) - Flow pathways and velocity - Saturation - Colloid concentration	2,5

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.09.59	Sorption of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	- Surface complexation properties - Flow pathways and velocity - Saturation - Colloid concentration [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	2,5
2.1.09.60	Sorption of Colloids at Air-Water Interface in EBS		2,5
2.1.09.61	Filtration of Colloids in EBS	- Physical filtration (dependent on flow pathways, colloid size)- Electrostatic filtration	2,5
2.1.09.62	Radionuclide Transport Through Liners and Seals	- Advection - Dispersion - Diffusion - Sorption [contributes to Radionuclide release from EBS in 2.1.09.63]	5
2.1.09.63	Radionuclide Release from the EBS - Dissolved - Colloidal - Gas Phase	- Spatial and temporal distribution of releases to the host rock (due to varying flow pathways and velocities, varying component degradation rates, varying transport properties) [contributions from Dissolved in 2.1.09.51/52/53, Colloidal in 2.1.09.57/58/59, Gas Phase in 2.1.12.03, Liners and Seals in 2.1.09.62]	5
2.1.10.00	1.10. BIOLOGICAL PROCESSES		
2.1.10.01	Microbial Activity in EBS - Natural - Anthropogenic	- Effects on corrosion - Formation of complexants - Formation of microbial colloids - Formation of biofilms - Biodegradation - Biomass production - Bioaccumulation [see also Microbially Influenced Corrosion in 2.1.03.06, Complexation in EBS in 2.1.09.54, Radiological Mutation of Microbes in 2.1.13.03]	2,5
2.1.11.00	1.11. THERMAL PROCESSES		
2.1.11.01	Heat Generation in EBS	- Heat transfer (spatial and temporal distribution of temperature and relative humidity) [see also Thermal-Hydrologic Effects from Preclosure in 1.1.02.03, Waste Inventory in 2.1.01.01]	2,4,5
2.1.11.02	Exothermic Reactions in EBS	- Oxidation of SNF - Hydration of concrete	4,5

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.11.03	Effects of Backfill on EBS Thermal Environment	- Thermal blanket - Condensation	4
2.1.11.04	Effects of Drift Collapse on EBS Thermal Environment	- Thermal blanket - Condensation	3,4
2.1.11.05	Effects of Influx (Seepage) on Thermal Environment	- Temperature and relative humidity (spatial and temporal distribution) [see also Influx/Seepage into EBS in 2.1.08.09]	4
2.1.11.06	Thermal-Mechanical Effects on Waste Form and In-Package EBS Components	- Alteration - Cracking - Thermal expansion / stress	2,3
2.1.11.07	Thermal-Mechanical Effects on Waste Packages	- Thermal sensitization / phase changes - Cracking - Thermal expansion / stress / creep	2,3
2.1.11.08	Thermal-Mechanical Effects on Backfill	- Alteration - Cracking - Thermal expansion / stress	3
2.1.11.09	Thermal-Mechanical Effects on Other EBS Components - Seals - Liner / Rock Reinforcement Materials - Waste Package Support Structure	- Alteration - Cracking - Thermal expansion / stress	3
2.1.11.10	Thermal Effects on Flow in EBS	- Altered influx/seepage - Altered saturation / relative humidity (dry-out, resaturation) - Condensation	4
2.1.11.11	Thermally-Driven Flow (Convection) in EBS	- Convection	4
2.1.11.12	Thermally-Driven Buoyant Flow / Heat Pipes in EBS	- Vapor flow	4
2.1.11.13	Thermal Effects on Chemistry and Microbial Activity in EBS		1,2,5
2.1.11.14	Thermal Effects on Transport in EBS	- Thermal diffusion (Soret effect) - Thermal osmosis	5
2.1.12.00	1.12. GAS SOURCES AND EFFECTS		
2.1.12.01	Gas Generation in EBS	- Repository Pressurization - Mechanical Damage to EBS Components - He generation from waste from alpha decay - H ₂ generation from waste package corrosion - CO ₂ , CH ₄ , and H ₂ S generation from microbial degradation -	2,3,4

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.1.12.02	Effects of Gas on Flow Through the EBS	- Two-phase flow - Gas bubbles [see also Buoyant Flow/Heat Pipes in 2.1.11.12]	4
2.1.12.03	Gas Transport in EBS	- Gas phase transport - Gas phase release from EBS	5
2.1.12.04	Gas Explosions in EBS	[see also Flammable Gas from Waste in 2.1.02.05]	3,5
2.1.13.00	1.13. RADIATION EFFECTS		
2.1.13.01	Radiolysis - In Waste Package - In Backfill - In Tunnel	- Gas generation - Altered water chemistry	1,2
2.1.13.02	Radiation Damage to EBS Components - Waste Form - Waste Package - Backfill - Other EBS Components	- Enhanced waste form degradation - Enhanced waste package degradation - Enhanced backfill degradation - Enhanced degradation of other EBS components (liner/rock reinforcement materials, seals, waste support structure)	2,3
2.1.13.03	Radiological Mutation of Microbes		5
2.1.14.00	1.14. NUCLEAR CRITICALITY		
2.1.14.01	Criticality In-Package	- Formation of critical configuration	2
2.1.14.02	Criticality in EBS or Near-Field	- Formation of critical configuration	5
2.2.00.00	2. GEOLOGICAL ENVIRONMENT		
2.2.01.00	2.01. EXCAVATION DISTURBED ZONE (EDZ)		
2.2.01.01	Evolution of EDZ	- Lateral extent, heterogeneities - Physical properties - Flow pathways - Chemical characteristics of groundwater in EDZ - Radionuclide speciation and solubility in EDZ - Thermal-mechanical effects - Thermal-chemical alteration [see also Mechanical Effects of Excavation in 1.1.02.02]	3,4,5

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.2.02.00	2.02. HOST ROCK		
2.2.02.01	Stratigraphy and Properties of Host Rock	<ul style="list-style-type: none"> - Rock units - Thickness, lateral extent, heterogeneities, discontinuities, contacts - Physical properties - Flow pathways <p>[see also Fractures in 2.2.05.01 and Faults in 2.2.05.02]</p>	N/A
2.2.03.00	2.03. OTHER GEOLOGIC UNITS		
2.2.03.01	Stratigraphy and Properties of Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	<ul style="list-style-type: none"> - Rock units - Thickness, lateral extent, heterogeneities, discontinuities, contacts - Physical properties - Flow pathways <p>[see also Fractures in 2.2.05.01 and Faults in 2.2.05.02]</p>	N/A
2.2.05.00	2.05. FLOW AND TRANSPORT PATHWAYS		
2.2.05.01	Fractures - Host Rock - Other Geologic Units	<ul style="list-style-type: none"> - Rock properties <p>[see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01]</p>	N/A
2.2.05.02	Faults - Host Rock - Other Geologic Units	<ul style="list-style-type: none"> - Rock properties <p>[see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01]</p>	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.2.05.03	Alteration and Evolution of Geosphere Flow Pathways - Host Rock - Other Geologic Units	<ul style="list-style-type: none"> - Changes In rock properties - Changes in faults - Changes in fractures - Plugging of flow pathways - Changes in saturation <p>[see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01, Fractures in 2.2.05.01, and Faults in 2.2.05.02]</p> <p>[see also Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07]</p>	N/A
2.2.07.00	2.07. MECHANICAL PROCESSES		
2.2.07.01	Mechanical Effects on Host Rock	<ul style="list-style-type: none"> - From subsidence - From salt creep - From clay deformation - From granite deformation (rockfall / drift collapse into tunnels) - Chemical precipitation / dissolution - Stress regimes <p>[see also Subsidence in 1.2.02.01, Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07]</p>	N/A
2.2.07.02	Mechanical Effects on Other Geologic Units	<ul style="list-style-type: none"> - From subsidence - Chemical precipitation / dissolution - Stress regimes <p>[see also Subsidence in 1.2.02.01, Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07]</p>	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.2.08.00	2.08. HYDROLOGIC PROCESSES		
2.2.08.01	Flow Through the Host Rock	<ul style="list-style-type: none"> - Saturated flow - Fracture flow / matrix imbibition - Unsaturated flow (fingering, capillarity, episodocity, perched water) - Preferential flow pathways - Density effects on flow - Flow pathways out of Host Rock <p>[see also Influx/Seepage into EBS in 2.1.08.09, Alteration of Flow Pathways in 2.2.05.03, Thermal Effects on Flow in 2.2.11.01, Effects of Gas on Flow in 2.2.12.02]</p>	N/A
2.2.08.02	Flow Through the Other Geologic Units - Confining units - Aquifers	<ul style="list-style-type: none"> - Saturated flow - Fracture flow / matrix imbibition - Unsaturated flow (fingering, capillarity, episodocity, perched water) - Preferential flow pathways - Flow pathways out of Other Geologic Units <p>[see also Alteration of Flow Pathways in 2.2.05.03, Thermal Effects on Flow in 2.2.11.01, Effects of Gas on Flow in 2.2.12.02]</p>	N/A
2.2.08.03	Effects of Recharge on Geosphere Flow - Host Rock - Other Geologic Units	<ul style="list-style-type: none"> - Infiltration rate - Water table rise/decline <p>[see also Infiltration in 2.3.08.03]</p>	N/A
2.2.08.04	Effects of Repository Excavation on Flow Through the Host Rock	<ul style="list-style-type: none"> - Saturated flow (flow sink) - Unsaturated flow (capillary diversion, drift shadow) - Influx/Seepage into EBS (film flow, enhanced seepage) <p>[see also Influx/Seepage into EBS in 2.1.08.09]</p>	3,4
2.2.08.05	Condensation Forms in Host Rock	<ul style="list-style-type: none"> - Condensation cap - Shedding <p>[see also Thermal Effects on Flow in Geosphere in 2.2.11.01]</p>	4
2.2.08.06	Flow Through EDZ	<ul style="list-style-type: none"> - Saturated / Unsaturated flow - Fracture / Matrix flow 	4

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.2.08.07	Mineralogic Dehydration	- Dehydration reactions release water and may lead to volume changes	N/A
2.2.08.08	Groundwater Discharge to Biosphere Boundary	- Surface discharge (water table, capillary rise, surface water) - Flow across regulatory boundary	N/A
2.2.08.09	Groundwater Discharge to Well	- Human use (drinking water, bathing water, industrial) - Agricultural use (irrigation, animal watering)	N/A
2.2.09.00	2.09.CHEMICAL PROCESSES - CHEMISTRY		
2.2.09.01	Chemical Characteristics of Groundwater in Host Rock	- Water composition (radionuclides, dissolved species, ...) - Water chemistry (temperature, pH, Eh, ionic strength ...) - Reduction-oxidation potential - Reaction kinetics - Interaction with EBS - Interaction with host rock [see also Chemistry in Tunnels in 2.1.09.04, Chemical Interactions and Evolution in 2.2.09.03] [contributes to Chemistry of Water Flowing into Repository in 2.1.09.01]	1
2.2.09.02	Chemical Characteristics of Groundwater in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	- Water composition (radionuclides, dissolved species, ...) - Water chemistry (temperature, pH, Eh, ionic strength ...) - Reduction-oxidation potential - Reaction kinetics - Interaction with other geologic units [see also Chemical Interactions and Evolution in 2.2.09.04]	1
2.2.09.03	Chemical Interactions and Evolution of Groundwater in Host Rock	- Host rock composition and evolution (granite, clay, salt ...) - Evolution of water chemistry in host rock - Chemical effects on density - Interaction with EBS - Reaction kinetics - Mineral dissolution/precipitation - Redissolution of precipitates after dry-out [contributes to Chemistry in Host Rock in 2.2.09.01]	1

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.2.09.04	Chemical Interactions and Evolution of Groundwater in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	- Host rock composition and evolution (granite, clay, salt ...) - Evolution of water chemistry in host rock - Chemical effects on density - Reaction kinetics - Mineral dissolution/precipitation - Recharge chemistry [contributes to Chemistry in Other Geologic Units in 2.2.09.02]	1
2.2.09.05	Radionuclide Speciation and Solubility in Host Rock	- Dissolved concentration limits [controlled by Chemistry in Host Rock in 2.2.09.01]	1
2.2.09.06	Radionuclide Speciation and Solubility in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	- Dissolved concentration limits [controlled by Chemistry in Other Geologic Units in 2.2.09.02]	1
2.2.09.50	2.09. CHEMICAL PROCESSES - TRANSPORT		
2.2.09.51	Advection of Dissolved Radionuclides in Host Rock	- Flow pathways and velocity - Advective properties (porosity, tortuosity) - Dispersion - Matrix diffusion - Saturation [see also Gas Phase Transport in 2.2.12.03]	N/A
2.2.09.52	Advection of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	- Flow pathways and velocity - Advective properties (porosity, tortuosity) - Dispersion - Matrix diffusion - Saturation [see also Gas Phase Transport in 2.2.12.03]	N/A
2.2.09.53	Diffusion of Dissolved Radionuclides in Host Rock	- Gradients (concentration, chemical potential) - Diffusive properties (diffusion coefficients) - Flow pathways and velocity - Saturation	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.2.09.54	Diffusion of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	- Gradients (concentration, chemical potential) - Diffusive properties (diffusion coefficients) - Flow pathways and velocity - Saturation	N/A
2.2.09.55	Sorption of Dissolved Radionuclides in Host Rock	- Surface complexation properties - Flow pathways and velocity - Saturation [see also Chemistry in Host Rock in 2.2.09.01]	N/A
2.2.09.56	Sorption of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	- Surface complexation properties - Flow pathways and velocity - Saturation [see also Chemistry in Host Rock in 2.2.09.01] -	N/A
2.2.09.57	Complexation in Host Rock	- Presence of organic complexants (humates, fulvates, carbonates, ...) - Enhanced transport of radionuclides associated with organic complexants	N/A
2.2.09.58	Complexation in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	- Presence of organic complexants (humates, fulvates, carbonates, ...) - Enhanced transport of radionuclides associated with organic complexants	N/A
2.2.09.59	Colloidal Transport in Host Rock	- Flow pathways and velocity - Saturation - Advection - Dispersion - Diffusion - Sorption - Colloid concentration	N/A
2.2.09.60	Colloidal Transport in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	- Flow pathways and velocity - Saturation - Advection - Dispersion - Diffusion - Sorption - Colloid concentration	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.2.09.61	Radionuclide Transport Through EDZ	<ul style="list-style-type: none"> - Advection - Dispersion - Diffusion - Sorption 	5
2.2.09.62	Dilution of Radionuclides in Groundwater - Host Rock - Other Geologic Units	<ul style="list-style-type: none"> - Mixing with uncontaminated groundwater - Mixing at withdrawal well [see also Groundwater Discharge to Well in 2.2.08.09]	N/A
2.2.09.63	Dilution of Radionuclides with Stable Isotopes - Host Rock - Other Geologic Units	<ul style="list-style-type: none"> - Mixing with stable and/or naturally occurring isotopes of the same element 	N/A
2.2.09.64	Radionuclide Release from Host Rock - Dissolved - Colloidal - Gas Phase	<ul style="list-style-type: none"> - Spatial and temporal distribution of releases to the Other Geologic Units (due to varying flow pathways and velocities, varying transport properties) [contributions from Dissolved in 2.2.09.51/53/55, Colloidal in 2.2.09.59, Gas Phase in 2.2.12.03, EDZ in 2.2.09.61]	N/A
2.2.09.65	Radionuclide Release from Other Geologic Units - Dissolved - Colloidal - Gas Phase	<ul style="list-style-type: none"> - Spatial and temporal distribution of releases to the Biosphere (due to varying flow pathways and velocities, varying transport properties) [see also Groundwater Discharge to Biosphere Boundary in 2.2.08.08, Groundwater Discharge to Well in 2.2.08.09, Recycling of Accumulated Radionuclides in 2.3.09.55] [contributions from Dissolved in 2.2.09.52/54/56, Colloidal in 2.2.09.60, Gas Phase in 2.2.12.03]	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.2.10.00	2.10. BIOLOGICAL PROCESSES		
2.2.10.01	Microbial Activity in Host Rock	<ul style="list-style-type: none"> - Formation of complexants - Formation and stability of microbial colloids - Biodegradation - Bioaccumulation <p>[see also Complexation in Host Rock in 2.2.09.57]</p>	N/A
2.2.10.02	Microbial Activity in Other Geologic Units (Non-Host-Rock) <ul style="list-style-type: none"> - Confining units - Aquifers 	<ul style="list-style-type: none"> - Formation of complexants - Formation and stability of microbial colloids - Biodegradation - Bioaccumulation <p>[see also Complexation in Other Geologic Units in 2.2.09.58]</p>	N/A
2.2.11.00	2.11. THERMAL PROCESSES		
2.2.11.01	Thermal Effects on Flow in Geosphere <ul style="list-style-type: none"> - Repository-Induced - Natural Geothermal 	<ul style="list-style-type: none"> - Altered saturation / relative humidity (dry-out, resaturation) - Altered gradients, density, and/or flow pathways - Vapor flow - Condensation 	N/A
2.2.11.02	Thermally-Driven Flow (Convection) in Geosphere	- Convection	N/A
2.2.11.03	Thermally-Driven Buoyant Flow / Heat Pipes in Geosphere	- Vapor flow	N/A
2.2.11.04	Thermal Effects on Chemistry and Microbial Activity in Geosphere	<ul style="list-style-type: none"> - Mineral precipitation / dissolution - Altered solubility <p>[contributes to Chemistry in 2.2.09.01 and 2.2.09.02]</p>	1
2.2.11.05	Thermal Effects on Transport in Geosphere	<ul style="list-style-type: none"> - Thermal diffusion (Soret effect) - Thermal osmosis 	N/A
2.2.11.06	Thermal-Mechanical Effects on Geosphere	<ul style="list-style-type: none"> - Thermal expansion / compression - Altered properties of fractures, faults, rock matrix 	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.2.11.07	Thermal-Chemical Alteration of Geosphere	<ul style="list-style-type: none"> - Mineral precipitation / dissolution - Altered properties of fractures, faults, rock matrix - Alteration of minerals / volume changes - Formation of near-field chemically altered zone (rind) 	N/A
2.2.12.00	2.12. GAS SOURCES AND EFFECTS		
2.2.12.01	Gas Generation in Geosphere	<ul style="list-style-type: none"> - Degassing (clathrates, deep gases) - Microbial degradation of organics 	N/A
2.2.12.02	Effects of Gas on Flow Through the Geosphere	<ul style="list-style-type: none"> - Altered gradients and/or flow pathways - Vapor/air flow - Two-phase flow - Gas bubbles <p>[see also Buoyant Flow/Heat Pipes in 2.2.11.03]</p>	N/A
2.2.12.03	Gas Transport in Geosphere	<ul style="list-style-type: none"> - Gas phase transport - Gas phase release from Geosphere 	N/A
2.2.14.00	2.14. NUCLEAR CRITICALITY		
2.2.14.01	Criticality in Far-Field	<ul style="list-style-type: none"> - Formation of critical configuration 	N/A
2.3.00.00	3. SURFACE ENVIRONMENT		
2.3.01.00	3.01. SURFACE CHARACTERISTICS		
2.3.01.01	Topography and Surface Morphology	<ul style="list-style-type: none"> - Recharge and discharge areas 	N/A
2.3.02.01	Surficial Soil Type	<ul style="list-style-type: none"> - Physical and chemical attributes 	N/A
2.3.04.01	Surface Water	<ul style="list-style-type: none"> - Lakes, rivers, springs - Dams, reservoirs, canals, pipelines - Coastal and marine features - Water management activities 	N/A
2.3.05.01	Biosphere Characteristics	<ul style="list-style-type: none"> - Climate - Soils - Flora and fauna - Microbes - Evolution of biosphere (natural, anthropogenic – e.g., acid rain) <p>[see also Climate in 1.3.01.01, Surficial Soil Type in 2.3.02.01, Microbial Activity in 2.3.10.01]</p>	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.3.07.00	3.07. MECHANICAL PROCESSES		
2.3.07.01	Erosion	<ul style="list-style-type: none"> - Weathering - Denudation - Subsidence <p>[see also Subsidence in 1.2.02.01, Periglacial Effects in 1.3.04.01, Glacial Effects in 1.3.05.01, Surface Runoff in 2.3.08.02, and Soil and Sediment Transport in 2.3.09.53]</p>	N/A
2.3.07.02	Deposition	- Weathering	N/A
2.3.07.03	Animal Intrusion into Repository		N/A
2.3.08.00	3.08. HYDROLOGIC PROCESSES		
2.3.08.01	Precipitation	<ul style="list-style-type: none"> - Spatial and temporal distribution <p>[see also Climate Change in 1.3.01.01] [contributes to Infiltration in 2.3.08.03]</p>	N/A
2.3.08.02	Surface Runoff and Evapotranspiration	<ul style="list-style-type: none"> - Runoff, impoundments, flooding, increased recharge - Evaporation - Transpiration (root uptake) <p>[see also Climate Change in 1.3.01.01, Erosion in 2.3.07.01] [contributes to Infiltration in 2.3.08.03]</p>	N/A
2.3.08.03	Infiltration and Recharge	<ul style="list-style-type: none"> - Spatial and temporal distribution - Effect on hydraulic gradient - Effect on water table elevation <p>[see also Topography in 2.3.01.01, Surficial Soil Type in 2.3.01.02] [contributes to Effects of Recharge in 2.2.08.03]</p>	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.3.09.00	3.09. CHEMICAL PROCESSES - CHEMISTRY		
2.3.09.01	Chemical Characteristics of Soil and Surface Water	<ul style="list-style-type: none"> - Altered recharge chemistry (natural) - Altered recharge chemistry (anthropogenic – e.g., acid rain) <p>[contributes to Chemical Evolution of Groundwater in 2.2.09.04]</p>	1
2.3.09.02	Radionuclide Speciation and Solubility in Biosphere	- Dissolved concentration limits	1
2.3.09.03	Radionuclide Alteration in Biosphere	<ul style="list-style-type: none"> - Altered physical and chemical properties - Isotopic dilution 	N/A
2.3.09.50	3.09. CHEMICAL PROCESSES - TRANSPORT		
2.3.09.51	Atmospheric Transport Through Biosphere	<ul style="list-style-type: none"> - Radionuclide transport in air, gas, vapor, particulates, aerosols - Processes include: wind, plowing, irrigation, degassing, saltation, precipitation 	N/A
2.3.09.52	Surface Water Transport Through Biosphere	<ul style="list-style-type: none"> - Radionuclide transport and mixing in surface water - Processes include: lake mixing, river flow, spring discharge, aeration, sedimentation, dilution <p>[see also Surface Water in 2.3.04.01]</p>	N/A
2.3.09.53	Soil and Sediment Transport Through Biosphere	<ul style="list-style-type: none"> - Radionuclide transport in on soil and sediments - Processes include: fluvial (runoff, river flow), eolian (wind), glaciation, bioturbation (animals) <p>[see also Erosion in 2.3.07.01, Deposition in 2.3.07.02]</p>	N/A
2.3.09.54	Radionuclide Accumulation in Soils	<ul style="list-style-type: none"> - Leaching/evaporation from discharge (well, groundwater upwelling) - Deposition from atmosphere or water (irrigation, runoff) 	N/A
2.3.09.55	Recycling of Accumulated Radionuclides from Soils to Groundwater	[see also Radionuclide Release in 2.2.09.65]	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
2.3.10.00	3.10. BIOLOGICAL PROCESSES		
2.3.10.01	Microbial Activity in Biosphere	- Effect on biosphere characteristics - Effect on transport through biosphere	N/A
2.3.11.00	3.11. THERMAL PROCESSES		
2.3.11.01	Effects of Repository Heat on Biosphere		N/A
2.4.00.00	4. HUMAN BEHAVIOR		
2.4.01.00	4.01. HUMAN CHARACTERISTICS		
2.4.01.01	Human Characteristics	- Physiology - Metabolism - Adults, children [contributes to Radiological Toxicity in 3.3.06.02]	N/A
2.4.01.02	Human Evolution	- Changing human characteristics - Sensitization to radiation - Changing lifestyle	N/A
2.4.04.00	4.04. LIFESTYLE		
2.4.04.01	Human Lifestyle	- Diet and fluid intake (food, water, tobacco/drugs, etc.) - Dwellings - Household activities - Leisure activities [see also Land and Water Use in 2.4.08.01] [contributes to Ingestion in 3.3.04.01, Inhalation in 3.3.04.02, External Exposure in 3.3.04.03]	N/A
2.4.08.00	4.08. LAND AND WATER USE		
2.4.08.01	Land and Water Use	- Agricultural (irrigation, plowing, fertilization, crop storage, greenhouses, hydroponics) - Farms and Fisheries (feed, water, soil) - Urban / Industrial (development, energy production, earthworks, population density) - Natural / Wild (grasslands, forests, bush, surface water)	N/A
2.4.08.02	Evolution of Land and Water Use	- New practices (agricultural, farming, fisheries) - Technological developments - Social developments (new/expanded communities)	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
3.0.00.00	3. RADIONUCLIDE / CONTAMINANT FACTORS (BIOSPHERE)		
3.1.00.00	1. CONTAMINANT CHARACTERISTICS		
3.2.00.00	2. RELEASE / MIGRATION FACTORS		
3.3.00.00	3. EXPOSURE FACTORS		
3.3.01.00	3.01. RADIONUCLIDE / CONTAMINANT CONCENTRATIONS		
3.3.01.01	Radionuclides in Biosphere Media	<ul style="list-style-type: none"> - Soil - Surface Water - Air - Plant Uptake - Animal (Livestock, Fish) Uptake <p>[contributions from Radionuclide Release from Geologic Units in 2.2.09.65, Transport Through Biosphere in 2.3.09.51/52/53/54/55]</p>	N/A
3.3.01.02	Radionuclides in Food Products	<ul style="list-style-type: none"> - Diet and fluid sources (location, degree of contamination, dilution with uncontaminated sources) - Foodstuff and fluid processing and preparation (water filtration, cooking techniques) <p>[see also Land and Water Use in 2.4.08.01, Radionuclides in Biosphere Media in 3.3.01.01]</p>	N/A
3.3.01.03	Radionuclides in Non-Food Products	<ul style="list-style-type: none"> - Dwellings (location, building materials and sources, fuel sources) - Household products (clothing and sources, furniture and sources, tobacco, pets) - Biosphere media <p>[see also Land and Water Use in 2.4.08.01, Radionuclides in Biosphere Media in 3.3.01.01]</p>	N/A
3.3.04.00	3.04. EXPOSURE MODES		
3.3.04.01	Ingestion	<ul style="list-style-type: none"> - Food products - Soil, surface water 	N/A
3.3.04.02	Inhalation	<ul style="list-style-type: none"> - Gases and vapors - Suspended particulates (dust, smoke, pollen) 	N/A
3.3.04.03	External Exposure	<ul style="list-style-type: none"> - Non-Food products - Soil, surface water 	N/A

Table A-1. Features, Events, and Processes (FEPs) Potentially Relevant to the Waste IPSC (continued)

UFD FEP Number	Description	Associated Processes	Challenge Milestone
3.3.06.00	3.06. TOXICITY / EFFECTS		
3.3.06.01	Radiation Doses	<ul style="list-style-type: none"> - Exposure rates (ingestion, inhalation, external exposure) - Dose conversion factors - Gases and vapors Suspended particulates (dust, smoke, pollen) 	N/A
3.3.06.02	Radiological Toxicity and Effects	- Human health effects from radiation doses	N/A
3.3.06.03	Non-Radiological Toxicity and Effects	- Human health effects from non-radiological toxicity	N/A

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