Generic Natural System Conceptual Model and Numerical Architecture – FY2012 Status Report

Fuel Cycle Research & Development

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U.S. Department of Energy
Used Fuel Disposition Campaign
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ACRONYMS

ADE	Advection – Dispersion Equation
EBS	Engineered Barrier System
EDZ	Engineered Disturbed Zone
FEPs	Features, Events, and Processes
GDSM	Generic Disposal System Model
HLW	High-Level Waste
LTHLW	Lower Than High-Level Waste
MIT	Massachusetts Institute of Technology
NEA	Nuclear Energy Agency
TSPA	Total System Performance Assessment
UFDC	Used Fuel Disposition Campaign
UNF	Used Nuclear Fuel
WIPP	Waste Isolation Pilot Plant
YMP	Yucca Mountain Project

USED FUEL DISPOSITION CAMPAIGN: GENERIC NATURAL SYSTEM CONCEPTUAL MODEL AND NUMERICAL ARCHITECTURE – FY2012 STATUS REPORT

1. INTRODUCTION

The Generic Disposal System Model (GDSM) is being developed and refined for use in performance assessment calculations of alternative disposal systems in clay, granite, salt, and deep boreholes. The natural system component of the GDSM must be comprehensive in the conceptual and numerical representation of features, events, and processes (FEPs) that are relevant to the four alternative disposal systems. In addition, the natural system component of the GDSM must be sufficiently flexible to accommodate differences among the disposal alternatives, while using a common, numerically efficient numerical architecture. This report develops a generic conceptual model of FEPs in the far field for use in the GDSM, lays out the mathematical governing equations for these FEPs, and determines a preliminary flexible numerical architecture for implementing the mathematical model of groundwater flow and radionuclide transport. In addition, the generic conceptual model is expressed as reference conceptual models for each of the four disposal system alternatives.

1.1 Generic Disposal System Modeling Objectives

The overarching goal of this report is to provide the conceptual basis for the natural system component of the GDSM and provide guidance on the numerical implementation of that component in the next-generation of the GDSM. Individual objectives of this activity include:

- A review the FEPs that have been identified as relevant to the four alternative disposal systems and a determination those that must be included in the conceptual model of the generic natural system component of the GDSM
- An identification and listing of the mathematical models for groundwater flow, radionuclide transport, and interrelated processes in the natural system, including alternative mathematical representations of the relevant FEPs
- An articulation of reference conceptual models for the four alternative disposal systems that can be used as the basis for numerical models of the natural system for incorporation in the GDSM
- An exploration of alternative strategies for the numerical implementation of flow and transport in the generic natural system model and determination of a preliminary numerical architecture for implementation in the GDSM
- A treatment of FEPs, conceptual models, and interfaces that is consistent with other components of the GDSM, in particular, the engineered barrier system (EBS).

1.2 Generic Natural System Model Requirements

As a component of the GDSM, the natural system model must meet a set of requirements based on the nature and intended use of the GDSM. The goal of the GDSM is to provide information on postclosure risk for alternative disposal environments and waste form options during future phases of the Used Fuel Disposition Campaign (UFDC), including (1) viability, (2) screening, (3) site selection, (4) characterization / engineering design, and (5) licensing (Clayton et al., 2011). The GDSM is also used to prioritize research and development needs. The GDSM is intended to take a holistic approach to system modeling in which alternative disposal system concepts are incorporated into a single modeling framework. It is also considered desirable to minimize the abstraction and external execution of component models for the GDSM; i.e., it is a goal to fully incorporate component, subsystem models into the execution of the GDSM. Full integration of subsystem models into the GDSM will enhance the transparency and traceability of postclosure risk analyses, and provide augmented quality assurance control over simulation results.

The basic requirements of the generic natural system model are generally shared with other component models of the GDSM, and include:

- Inclusive: The generic natural system model must include all FEPs relevant to postclosure repository performance and these FEPs must be assembled into a coherent conceptual model of the natural system. Relevant FEPs consist of all FEPs that have been deemed as included, or potentially included, in the FEPs screening process. If a particular FEP is screened in for any of the alternative disposal systems, then functionality for that FEP must be included in the generic natural system model. It may also be desirable to include numerical functionality for some FEPs that have been screened out as excluded, for the purpose of demonstrating low consequences of that FEP or for consideration of alternative conceptual models. Previous FEPs screening activities for the Yucca Mountain Project (YMP) have used analyses and models other than the Total System Performance Assessment (TSPA) model to justify a low-consequence determination for many excluded FEPs. Although this and a wide range of approaches to FEPs screening are valid (PAMINA 2011), a FEPs screening process that uses system-level modeling is less subjective than expert judgments or separate analyses, and may be preferable. This implies that it would be better to include key excluded FEPs in the system model, even if those FEPs are ultimately excluded from the TSPA model.
- Comprehensive: Based on the desire to limit the use of conservative assumptions or model abstractions in the GDSM, the generic natural system model should be comprehensive in its capabilities. An important example of comprehensiveness is radionuclide transport simulation for all radionuclides in decay chains. The use of conservative assumptions of secular equilibrium and pre-decay “boosting” for some decay chain members should be avoided. Comprehensive incorporation of all radionuclides being transported in the natural system enhances clarity and realism of GDSM simulations.
- Flexible: The generic natural system model must be flexible enough to accommodate the four disposal system alternatives currently under consideration and potentially other future alternatives. This requirement includes flexibility with regard to variations in hydrogeologic units, structural geology, and boundary conditions associated with

alternatives. In addition, the generic natural system model must have the flexibility to handle differences in specific geologic media (e.g., porous versus fractured media) and in the processes related to groundwater flow and radionuclide transport (e.g., advectively dominated transport versus diffusion dominated transport). Ideally, the generic natural system model should have the flexibility of a set of switches built into the numerical framework that allow certain individual FEPs to be turned on or off, as needed, in the GDSM.

- Integrated with Other GDSM Components: The generic natural system model must be successfully integrated with other components of the GDSM with regard to the exchange of state variables, groundwater flow, radionuclide transport, geometric boundaries, model assumptions, numerical implementation, and values for common parameters. The interface with the generic EBS model is particularly critical and challenging. The nature of the coupling required between the generic natural system model and the generic EBS model varies from decoupled to fully coupled depending on the disposal system alternative and the process under consideration. For example, in a salt repository the negligible groundwater flow in the bedded salt of the EBS may be assumed to be decoupled from groundwater flow in overlying strata in the natural system. In a clay repository a unidirectional coupling for radionuclide transport may be assumed for diffusive migration of radionuclides from the EBS and clay into overlying and underlying more transmissive strata in the generic natural system model. In contrast, simulations of heat transport may require fully coupled, bidirectional coupling between the EBS and the natural system.

- Numerically Efficient: As a component of the GDSM, the generic natural system model must be capable of performing numerical simulations for multi-realization, Monte Carlo analyses within the computational budget of the GDSM. Numerous aspects of the generic natural system model impact the numerical performance of the model, including number of radionuclides tracked, number and complexity of processes simulated, coupling with other component models, heterogeneity of the system, grid resolution, time step size, and numerical methods used. Although exact constraints on the computational budget are difficult to determine *a priori*, the general requirement for numerical efficiency should be considered in development of the generic natural system model.

1.3 Four Disposal System Alternatives

The UFDC is conducting research on four basic disposal system alternatives for used nuclear fuel and high-level radioactive waste. These disposal concepts are (1) mined repository in salt, (2) mined repository in crystalline rock, (3) mined repository in clay, and (4) deep borehole disposal in crystalline rock. The geological media and conditions for each of these disposal system alternatives are defined in a broad sense, but are nonspecific with regard to detailed local geological or hydrogeological conditions. For example, a mined repository in salt could be in bedded salt or in a salt dome. Crystalline rock refers to a range of mineralogy and petrology among igneous and metamorphic rock types. Nonetheless, the basic characteristics of the four disposal systems are based on typical geological conditions associated with the corresponding host media and experience in these media in the United States and international repository science programs.

These four disposal system alternatives are among a broad range of options considered during the 1970s in the United States. A mined repository in salt, granite, or clay was considered to be the favored option at that time, with deep borehole disposal being less favorable because of drilling limitations using then-current technology. Subsequent advances in drilling technology have increased the viability of deep borehole disposal in crystalline rock. International and U.S. efforts have largely confirmed the potential viability of these disposal system alternatives. Safe disposal of non-heat generating radioactive waste has been demonstrated by the Waste Isolation Pilot Plant (WIPP) in the U.S. and research continues on used fuel disposal in salt domes in Germany. Disposal in crystalline rocks is under scientific investigation in Switzerland, Japan, and Korea, and has advanced to the stage of site selection and licensing in Sweden and Finland. Active research programs for disposal in clay exist in France, Switzerland, and Belgium. Investigation of the deep borehole disposal alternative generally has been limited to conceptual design studies, modeling, and literature investigations, but active research programs exist at the Massachusetts Institute of Technology (MIT) and at Sandia National Laboratories.

The salt repository disposal system concept consists of a mined repository excavated in bedded salt at a nominal depth of 500 m, similar to the WIPP disposal system. Although numerous alternatives exist for the details of waste emplacement, the repository is conceptualized to consist of multiple, approximately horizontal galleries in the salt. The natural system surrounding the repository is composed of the engineered disturbed zone (EDZ) in the salt, the bedded salt, underlying sedimentary strata, overlying sedimentary strata, and unconsolidated near-surface deposits. Groundwater in salt formations is generally present within intercrystalline porosity or fluid inclusions rather than as a continuous phase. Interconnected porosity may be present in fissures, faults and/or interbeds. Under natural stratification conditions, the permeability of rock salt is extremely low. Rock salt also exhibits a high level of specific thermal conductivity. Rock salt reacts to mechanical load with a slow, flowing movement that is known as “salt creep”. This particular property of rock salt causes cavities and fissures to be self-sealed over time. Bedded salt that has formed as evaporites in a sedimentary basin is geologically associated with fine-grained clastic sedimentary rocks. Underlying and Overlying sedimentary rocks may consist of a wide range of sedimentary rock types originating from active basinal filling, including shales, sandstones, and carbonates. An example of a lower than high-level waste (LTHLW) repository in a bedded salt is the DOE WIPP site (DOE 1996).

The crystalline rock repository disposal system entails a mined repository excavated in crystalline rock at a nominal depth of 500 m. Favorable crystalline rock types include granite, granitic gneiss, and other felsic igneous and metamorphic rock types. As with the other mined repository alternatives, the repository layout consists of multiple, approximately horizontal drifts. The natural system surrounding the repository includes the EDZ in the host rock, the underlying and overlying crystalline rock, and unconsolidated near-surface deposits. Naturally occurring fractures, faults, and shear zones constitute important features in crystalline rock with regard to groundwater flow and radionuclide transport. An example of a proposed UNF repository in saturated granite is the Swedish KBS-3 concept (SKB 2006).

The clay repository disposal system consists of a mined repository in clay, shale or argillite at a nominal depth of 500 m. The repository layout would consist of multiple, horizontal drifts in the clay host rock. The natural system includes the EDZ, the host rock, underlying and overlying sedimentary rocks, and unconsolidated near-surface deposits. Clay/shale formations have low permeability, plasticity, fracture sealing or healing, and high sorption capacity. Clay-rich deposits appropriate for used fuel disposal may be associated with a wide range of other overlying or underlying sedimentary rock types, including sandstones and carbonate rocks. Examples of proposed UNF and HLW repositories in saturated clays are the Swiss project in Opalinus Clay (NAGRA 2002) and the French project in Callovo-Oxfordian argillites (ANDRA 2005).

The deep borehole disposal concept involves drilling a borehole to a nominal depth of 5000 m into crystalline basement rocks and disposal of waste in the lower 2000 m of the borehole. The upper 3000 m of the borehole would be sealed in a manner similar to the sealing of boreholes and shafts in the shallower mined repository disposal systems. An array of multiple disposal boreholes would be developed at a given site. A summary of deep borehole disposal is presented in Brady et al. (2009) and reference conceptual design of the disposal system is described in Arnold et al. (2011) Favorable crystalline host rock types include granite, granitic gneiss, and other felsic igneous and metamorphic rock types. The natural system for the borehole disposal system is composed of the EDZ, the crystalline host rock, overlying crystalline rock and sedimentary strata, and unconsolidated near-surface deposits. Overlying sedimentary strata in stable, intracontinental geological settings favorable for deep borehole disposal would likely consist of a wide variety of generally horizontal strata, including shales, sandstones, and carbonates.

2. FEATURES, EVENTS, AND PROCESSES

2.1 Approach to Natural System FEPs Analysis

Previous work (Freeze et al. 2010) has identified 208 FEPs applicable to the range of waste types and disposal concepts/geologic settings analyzed for the UFDC. These FEPs were derived from FEP lists from 10 different national radioactive waste disposal programs available from the Nuclear Energy Agency (NEA) FEP database (NEA 1999; NEA 2006) and from the Yucca Mountain Project (YMP) FEP list (SNL 2008a; SNL 2008). The FEPs are applicable to 20 combinations of 5 disposal concepts/geologic settings and 4 waste form types.

The following 4 waste types were considered:

- Used Nuclear Fuel (UNF)
- High-Level Waste (HLW) Glass
- HLW Glass Ceramic / Ceramic
- HLW Metal Alloy

The 5 disposal concepts / geologic settings included:

- Mined Geologic Disposal (Hard Rock, Unsaturated)
- Mined Geologic Disposal (Hard Rock, Saturated), referred to as Granite
- Mined Geologic Disposal (Clay/Shale, Saturated), referred to as Clay
- Mined Geologic Disposal (Salt, Saturated), referred to as Salt
- Deep Borehole Disposal

Four disposal concepts/geologic settings are considered in this report (the unsaturated concept was excluded), as described in Section 1.3.

The FEPs list in Freeze et al. (2010) contains 51 FEPs applicable to the Natural Systems or "Geosphere". Unlike the EBS FEPs, the geosphere FEPs are not waste type specific. The same geosphere processes are applicable to the different types of wastes. Consequently, the number of possible combinations is equal to the number of the disposal concepts/geologic settings, which is equal to 4 times the number of natural system FEPs.

Note that the geosphere FEPs, as well as EBS and Biosphere FEPs, consider "nominal" conditions and do not include unlikely external factors. The FEPs are organized in the Freeze list such that factors such as seismic and igneous effects and human intrusion and their impact on the geosphere, EBS, and Biosphere are considered in the external category.

The geosphere consists of 3 components: the EDZ; Host Rocks; and Other Geologic Units. The EDZ is defined as a region around the repository mechanically disturbed by the stress caused by the presence of the excavation. Some FEPs are applicable only to one component, the others are applicable to 2 components, and a few are applicable to all 3 components. The EDZ and host rocks are disposal concepts/geologic settings specific. Consequently, each geosphere FEP related to EDZ and host rocks component has to be evaluated for the granite, clay, salt, and deep borehole systems. Note that the EDZ is the host rock with altered properties and properties that vary temporally over a short timescale relative to geologic or regulatory timeframes.

The other geologic units component consists of confining units; aquifer(s); and unsaturated units. These components are not disposal concept/geologic setting specific. Consequently, each geosphere FEP related to other geologic units component has to be evaluated for confining units, aquifer(s), and unsaturated units regardless of which disposal concept/setting it is related to.

Most of the FEPs include more than one process. A process may be applicable to one and not applicable to another disposal concept/geologic setting. Similarly, a process may be applicable to one component of the other geologic units and not applicable to another one.

The most important FEPs input into the generic natural system conceptual model consists of mapping geosphere FEPs and associated processes to the different geosphere components and sub-components for the different disposal concepts/geologic settings (if applicable). Because the disposal concepts/geologic settings are generic, the mapping can be done only at a high level and it is not intended to provide any specific details. At this high level of evaluation, a process is either considered to be applicable or not applicable. The not applicable processes also include the processes with low importance/low consequences. The applicable processes are categorized either as “very important” or “somewhat important”. The very important processes are those that need to be implemented in the generic natural system conceptual model. The importance is defined based on the capability of the process to facilitate or delay radionuclide transport and/or to enhance or diminish the component performance. The somewhat important processes may or may not be implemented in the generic natural system conceptual model. In the latter case, these processes may need to be either addressed in an alternative model or in an in-depth evaluation. In both cases, an adequate justification for excluding a specific somewhat important process should be provided.

The FEPs mapping is summarized in Table A-1 (Appendix A). The screening decisions provided in this table are largely based on the expert judgment of the authors of this report and on previous prioritization analyses in the UFDC Research and Development Roadmap (DOE, 2011). The brief review of each FEP is considered in Section 2.2. This review summarizes the most pertinent information that was used in making screening decision.

The UFD Roadmap provides the overall priority score for each FEP (Appendix B of DOE, 2011). The priority score is calculated based on FEP importance to safety case and importance to the decision scaled to account for the weight of each decision point. Four decision points were considered: (1) site screening; (2) site selection; (3) site characterization; and (4) site suitability. The weights were developed for each of these decision points.

Safety case importance is evaluated for each of three components: (1) safety assessment (IS_a); (2) design, construction, operation (IS_d); and (3) confidence (IS_c). The resulting importance is calculated as the sum of the product of each component importance (same for each decision point) and its weight (decision point specific). The weights were developed for each component and each decision point.

The importance to the decision in each decision point is evaluated based on the importance to the safety case and the need in supporting information, which can be not necessary (low importance to decision); supports or improve decision (medium importance to decision), and essential to the decision (high importance to decision). The maximum possible overall priority score based on this method is 13. The highest priority indicates that all 3 components of the safety case have high importance; the information is essential to the decision, and this information is currently insufficient and does not adequately represent specific FEPs. The highest overall priority score is 8 (Appendix B of DOE, 2011).

Because the UFD Road map priority scores combine multiple factors with different weights at the different decision points, it is not possible to conclude which of these factors are the greatest contributors to the priority. The safety case importance scores summarized in Appendix A of (DOE, 2011) are considered to be more useful scores for this FEP analysis.

To combine the importance to the different safety case components scores into one score for each FEP, the same approach as described in (DOE, 2011) was used. The overall importance to the safety case *IS* was calculated as:

$$\boldsymbol{IS = \sum_{k=1}^{4}[(IS_a \cdot w_{a,k} + IS_d \cdot w_{d,k} + IS_c \cdot w_{c,k}) \cdot \alpha_k]} \qquad \textbf{2-1}$$

where *k* represents a decision point.

The values for the importance to the safety case components IS_a, IS_d, and IS_c were taken from appendix A in (DOE, 2011). These values are either 1 (low importance), or 2 (medium importance), or 3 (high importance). The safety case component and decision point specific weights $w_{a,k}$ were taken from Table 2 in (DOE, 2011). The decision point specific weights α_k were taken from Table 5 in (DOE, 2011). Note, that *IS* values range from 1 to 3.

The *IS* values calculated using Equation (2-1) and the overall priority scores *P* from Appendix B in (DOE, 2011) are provided in Table A-1. Note that even though these scores were quantified, they are primarily based on the expert judgment. As it was pointed out in (DOE, 2011), "the scores can be changed to reflect differing priorities". The evaluation in (DOE, 2011) represented an important basis for this FEP analysis; however, some conclusions may differ from the ones in (DOE, 2011).

The brief review of each FEP is considered in Section 2.2. This review summarizes the most pertinent information that was used in making screening decision.

2.2 Review and Preliminary Screening of Natural System FEPs

The information presented in this section is substantially based on the evaluations in (Freeze et al. 2010). However, not all the geosphere FEPs were evaluated in (Freeze et al. 2010) and some evaluations are not complete or are limited to one disposal concept/geologic setting. In these cases, the other sources were used as indicated.

The intent of this section is to provide a brief description of each FEP with the focus on the facts and arguments that are of the greatest importance to the screening decision. The FEPs are considered in their numbering order. Note that this preliminary screening is not a formal FEPs screening and it is suitable for generic evaluations, which is appropriate for the early stage in the program. Additional justification would be required at the later stages when site specific information becomes available and the regulatory framework is defined.

2.2.01.01 Evolution of EDZ (IS=3, P=2.58 for granite and salt, 6.13 for deep borehole, and 8.0 for clay)

This FEP is applicable to EDZ. The following processes and features are included:

- 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

The excavation will result in both, mechanical and chemical disturbances in the EDZ. These disturbances will, to some degree, affect the EDZ properties. Of greatest concern is formation of new fractures and re-opening of existing fractures and micro-fracturing in EDZ because it may increase permeability and facilitate radionuclide transport.

Because the EDZ size is expected to be small compared to the spatial dimensions of the host rock, configuration of EDZ and other natural flow pathways, the processes related to this FEP should have moderate importance. The lateral extent, physical properties, and flow pathways are categorized as somewhat important for Granite, Clay, and Salt. The other processes for these concepts are considered to be of low importance.

For Deep Borehole, the lateral extent, physical properties, and flow pathways are categorized as very important. This is because the EDZ around the deep borehole may provide a direct flow and transport pathway (upwards and along the seal/EDZ interface which extends to the surface) to the exposure points. The thermal-mechanical effects are of some importance to the deep borehole because waste packages and thermal output are near the borehole wall in the deep borehole case.

2.2.02.01 Stratigraphy and Properties of Host Rock (IS=2.8, P=3.74)

This FEP is applicable to the host rocks. The following processes and features are included:

- Rock units
- Thickness, lateral extent, heterogeneities, discontinuities, contacts
- Physical properties
- Flow pathways

The stratigraphy of the host rocks is required to construct the geologic framework model, which represents one of the most important inputs into the simulations of the flow and radionuclide transport in the geosphere. The stratigraphic information should provide thickness and lateral extent of the host rocks and should be able to capture the major heterogeneities and discontinuities in the host rock properties.

The host rock properties have major impacts on the flow pathways and radionuclide transport regardless of the type of the disposal concept/geologic setting. All the processes associated with this FEP are assigned high importance for Granite, Clay, Salt, and Deep Borehole.

Note that this FEP does not consider issues related to the events and processes that may cause the physical properties of the host rocks to change over time. These changes are addressed in Alteration and Evolution of Geosphere Flow Pathways FEP (2.2.05.03).

2.2.03.01Stratigraphy and Properties of Other Geologic Units (IS=2.6, P=2.46)

This FEP is applicable to the other geologic units. The following processes and features are included:

- Rock units
- Thickness, lateral extent, heterogeneities, discontinuities, contacts
- Physical properties
- Flow pathways

The importance of the other geologic unit stratigraphy and properties is the same as the importance of the host rocks stratigraphy and properties. The other geologic units in most cases represent the pathway through which the radionuclides released from the host rocks are transported to the biosphere.

The other geologic unit properties have major impacts on the flow pathways and radionuclide transport. This especially concerns the properties of the confining units and aquifers. The properties of the unsaturated zone are of some importance because the major flow and transport pathways lay in the saturated zone.

Note that this FEP does not consider issues related to the events and processes that may cause the physical properties of the host rocks to change over time. These changes are addressed in Alteration and Evolution of Geosphere Flow Pathways FEP (2.2.05.03).

2.2.05.01 Fractures (IS=2.6, P=3.65)

This FEP is applicable to both, the host rocks and other geologic units. The following feature is included:

- Rock properties

Fractures in host rocks and other geologic units are important because they may significantly affect rock properties. The fracture properties are especially important for crystalline rocks because in these rocks the flow and transport occur mostly in the fractures. Consequently, the fractures are of high importance to the Granite and Deep Borehole disposal concepts (Deep Borehole is most likely to be located in crystalline basement rocks, such as granite).

The fractures in the other geologic units can be of some importance for an aquifer and unsaturated zone if these sub-components are in fractured rocks, whether these rocks are crystalline or other fractured rocks, such as carbonate sedimentary rocks. The fractures in the aquifer and unsaturated zone are of low importance in the case of porous media, such as alluvium.

The aquifer is the most common interface between the geosphere and biosphere when the exposure pathway is via use of contaminated groundwater. The unsaturated zone is an interface between the geosphere and biosphere when the exposure is via contaminated soil.

The fractures are of some importance to clay/shale because the fractures in these rocks may provide preferential flow and transport pathways and may facilitate radionuclide transport. This concerns both, the clay/shale as a host rock and the clay/shale as the other geologic units (confining unit sub-component).

Note that this FEP addresses the natural fractures under current, undisturbed conditions and does not consider the fractures induced or affected by natural seismic or igneous disruptive events that may occur in the future. The seismic and igneous events are considered in the External FEPs category.

The changes in fracture properties over time are addressed in FEP 2.2.05.03, Alteration and Evolution of Geosphere Flow Pathways.

2.2.05.02 Faults (IS is not available, P is not available)

This FEP is applicable to both, the host rock and other geologic units. The following process is included:

- Rock properties

This FEP is similar to the Fractures FEP because both fractures and faults affect rock properties in a similar way. Compared to fractures, faults tend to be more isolated, but they are more likely to be of a larger extent and to have long, spatially-correlated pathways cross-cutting multiple lithologic units. As with fractures, these pathways may have substantially higher permeability than the rock matrix and can serve as the preferential flow and transport pathways.

Faults are very common features in the crystalline rocks and because of that they are especially important for Granite and Deep Borehole. They have some importance for Clay and Salt. Faults can affect all sub-components related to the other geologic units regardless of whether these components are in fractured or porous media.

Note that this FEP is concerned exclusively with faults under current, undisturbed conditions. Similarly, this FEP does not address faults induced or affected by natural seismic or igneous disruptive events that may occur in the future.

The changes in fracture properties over time are addressed in FEP 2.2.05.03, Alteration and Evolution of Geosphere Flow Pathways.

2.2.05.03. Alteration and Evolution of Geosphere Flow Pathways (IS=1, P=2.46)

This FEP is applicable to both, the host Rock and other geologic units. The following processes are included:

- Changes in rock properties
- Changes in faults
- Changes in fractures
- Plugging of flow pathways
- Changes in saturation

This FEP addresses changes over time in rock properties, fractures, and faults that result from thermal, mechanical, and chemical effects of the repository on the host rocks and other geologic units. This FEP is closely related to Thermal-Mechanical Effects on Geosphere (FEP 2.2.11.06) and Thermal-Chemical Alteration of Geosphere (FEP 2.2.11.07).

The rock properties, fractures, and faults under the natural conditions are addressed in FEPs 2.2.02.01, 2.2.03.01, 2.2.05.01 and 2.2.05.02.

The changes due to tectonic, igneous, and geothermal processes, as well as sedimentation, erosion, glaciations, and fluid migration are addresses by the External FEPs.

Heat from the waste may cause thermal expansion of the surrounding rocks, generating changes in the stress field that may change the properties (both hydrologic and mechanical) of fractures in the rock. Cooling following the peak thermal period will also change the stress field, further affecting fracture properties near the repository. Thermal-mechanical effects are considered in FEP 2.2.11.06, Thermal-Mechanical Effects on Geosphere.

Thermal effects may impact radionuclide transport directly by causing changes in radionuclide speciation and solubility or, indirectly, by causing changes to host rock mineralogy that affect flow paths in the host rock. Relevant processes include precipitation and dissolution of fracture filling minerals and alteration of minerals. Thermal effects on chemical alteration are considered in FEP 2.2.11.07, Thermal-Chemical Alteration of Geosphere.

Chemical reactions can also result in gas generation. The gas can cause mechanical damage to the host rock, which in turn can result in pneumatic fracturing. Gas generation is specifically addressed in FEP 2.12.01, Gas Generation in Geosphere.

It is anticipated that Granite, Clay, and Salt repository designs will have thermal limits on the peak waste package temperature, although those limits may vary across these options. Maintaining these peak temperatures below the corresponding limits will result in moderate impacts on the temperatures of the host rocks and especially other geologic units and relatively short (compared to the regulatory period) time of thermal period.

The temperature limits are not applicable to the Deep Borehole. However, the zone of significant influence from the borehole will be smaller than the zone of influence from a repository.

As a result, this FEP is considered to be of low significance for both host rocks and other geologic units. However, THMC coupled process analyses may be needed on a case-by-case basis especially if site-specific conditions suggest that the changes in properties may extend beyond the thermal period.

2.2.07.01 Mechanical Effects on Host Rock (IS=3, P=1.63 for granite and deep borehole, P=3.83 for salt and clay)

This FEP is applicable to the host rocks. The following processes are included:

- Changes from subsidence
- Changes from salt creep
- Changes from clay deformation
- Changes from granite deformation (rockfall / drift collapse into tunnels)
- Chemical precipitation / dissolution
- Stress regimes

This FEP addresses mechanical effects caused by stresses induced by repository openings and thermal-hydrological-chemical processes associated with the repository, such as waste heat, potentially including boiling and condensation, dry-out and re-saturation. Chemical processes may result in gas generation that impacts the mechanical behavior. This FEP is closely related to Thermal-Mechanical Effects on Geosphere (FEP 2.2.11.06), Thermal-Chemical Alteration of Geosphere (FEP 2.2.11.07), and Gas Generation in Geosphere (FEP 2.12.01).

Mechanical effects can also be caused by diagenetic evolution of the host rock, as well as changes in regional stress, geothermal processes, erosion and glaciation, osmotic processes, and hydrocarbon, CO_2 or other geofluids that may migrate from some deeper source and interact with the host rock. These processes are addresses by the External FEPs.

Mechanical effects have low importance for Granite disposal concept. Clay deformation may be of some importance to Clay disposal concept. Salt creep process has some importance to Salt concept and stress regime has some importance to Deep Borehole concept.

2.2.07.02 Mechanical Effects on Other Geologic Units (IS=2, P=1.32 for granite and deep borehole, P=3.10 for salt and clay)

This FEP is applicable to the other geologic units. The following processes are included:

- Changes from subsidence
- Chemical precipitation / dissolution
- Stress regimes

The mechanical effects on the other geologic units are similar to the mechanical effects on the host rocks (FEP 2.2.07.01), except the magnitude of these effects is significantly lower due to the large distance between the other geologic units and repository.

The mechanical effects on the other geologic units are excluded based on low consequences.

2.2.08.01 Flow through the Host Rock (IS=2.6, P=0 for granite, 3.65 for clay and deep borehole, and 7.73 for salt)

This FEP is applicable to the host rocks. The following processes are included:

- Saturated flow
- Fracture flow / matrix imbibition
- Unsaturated flow (fingering, capillarity, episodicity, perched water)
- Preferential flow pathways
- Density effects on flow
- Flow pathways out of Host Rock

Under the saturated repository conditions, advective flow through the host rock is one of the most important pathways affecting radionuclide transport in geosphere. The advective flow is a function of hydraulic gradients and rock properties. The rock properties, fractures, and faults under the natural conditions are addressed in FEPs 2.2.02.01, 2.2.03.01, 2.2.05.01 and 2.2.05.02. The changes over time in rock properties, fractures, and faults that result from thermal, mechanical, and chemical effects of the repository are addressed in Alteration and Evolution of Geosphere Flow Pathways (FEP 2.2.05.03).

Advective flow is a dominant transport mechanism in fractured media and because of this it is especially important for Granite and Deep Borehole disposal concepts.

In the low permeability media, such as clay and shale, advective flow may be very slow. In these media diffusion is often considered to be the major transport mechanism. This assumption needs to be justified based on site-specific data.

A convenient way of comparing advective and diffusive flow is by using the Péclet number. The Péclet number is a dimensionless number that relates the effectiveness of mass transport by advection to the effectiveness of mass transport by either dispersion or diffusion. This number may also be thought of as the ratio between the advective and diffusive time scales. Generally, a Péclet number significantly smaller than 1 indicates that diffusion is dominant. Péclet numbers near 1 correspond to systems in which diffusion and advection are both important, and the values >10 relate to advection-dominated systems. Figure 1 shows the probability distribution of Péclet number in Callovo-Oxfordian argillites at the ANDRA site in Bure. The probability of having comparable advective and diffusive flow is 0.3. The probability of having dominant advective flow is small (0.05), but is not zero.

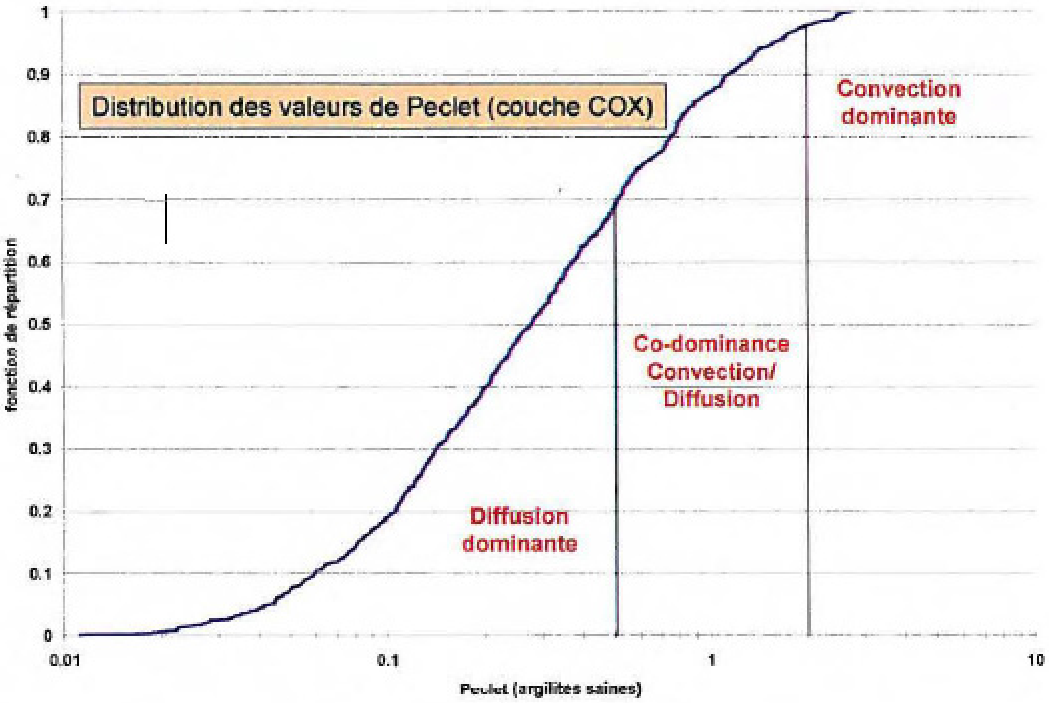


Figure 2-1. Probability Distribution of Péclet Number in Callovo-Oxfordian Argillite Formation (Figure 3.1-2 in C.RP.ACSS.05.0022).

Advective flow in low-permeability formations may have even greater importance in the case of fractures and faults. Both features may create preferential flow pathways.

Based on the information presented above, advective flow is assigned high importance for Granite and Deep Borehole concepts and some importance for Clay and Salt concepts.

Density effects on flow may occur due to heating from repository because higher groundwater temperatures will result in smaller densities. As a result, buoyancy will cause the higher temperature water to rise until temperature equilibrium is achieved. Due to moderate increase in temperatures and short duration of the thermal period compared to the regulatory period, the densities effects will be small. This effect is also considered in FEP 2.2.11.03, Thermally-Driven Buoyant Flow / Heat Pipes in Geosphere.

2.2.08.02 Flow through the Other Geologic Units (IS=2.6, P=0 for granite, 3.65 for clay and deep borehole, and 7.73 for salt)

This FEP is applicable to the other geologic units. The following processes are included:

- Saturated flow
- Fracture flow / matrix imbibition

- Unsaturated flow (fingering, capillarity, episodicity, perched water)
- Preferential flow pathways
- Density effects on flow
- Flow pathways out of Other Geologic Units

Flow through the other geologic units is the most important pathway through which the radionuclides released from the host rocks are transported to the biosphere. The type of flow will depend on the type of rocks. Confining units are low-permeability rocks. Consequently, the flow in these units will be a function of the same factors described for the clay/shale host rocks (FEP 2.2.08.01).

Flow in the aquifers is especially important because it affects the radionuclide concentrations in the groundwater well that directly affect the doses calculated by the biosphere model. The aquifers can be in both, porous or fractured media.

Some of the other geologic units above the repository may be partially in the unsaturated zone. Flow through the unsaturated zone may affect the water table and thus, the flow in an unconfined aquifer. These effects are also considered in Effects of Recharge on Geosphere Flow (FEP 2.2.08.03).

Preferential flow pathways might be of some importance to confining units. Preferential flow pathways in the unsaturated zone are of low importance because the major flow and transport pathways are in the saturated zone.

Flow pathways out of the other geologic units is are of high importance to all the components of the other geologic units because they affect the radionuclide transport to the exposure points.

2.2.08.03 Effects of Recharge on Geosphere Flow (IS is not available, P=0)

This FEP is applicable to both, host Rocks and the other geologic units. The following processes are included:

- Infiltration rate
- Water table rise/decline

Recharge is the flux of water into the saturated zone, following infiltration and percolation through the unsaturated zone. Recharge is a key factor that drives flow rates in the saturated zone as a function of space and time. Recharge directly affects the groundwater flow in an unconfined aquifer. Increased recharge will result in rising water table and in increased flow. Reduced recharge will cause the opposite effects.

Recharge will indirectly affect the other aquifers, confining units, host rocks, and EDZ because the changes in hydraulic heads in the unconfined aquifer will impact the hydraulic heads in all the systems. However, the magnitude of the impacts will be smaller and will decrease with depth.

Because recharge impacts the flow, it is related to FEPs 2.2.08.01, Flow through the Host Rock, 2.2.08.02, Flow through Other Geologic Units, and 2.2.08.06, Flow through EDZ.

The most common reason for changes in recharge is climate change. Recharge can be also affected by human activities. For example, irrigation may increase recharge beneath the irrigated fields.

Recharge is important to the other geologic units and has low importance to the host rocks and EDZ.

2.2.08.04 Effects of Repository Excavation on Flow through the Host Rock (IS=1.8, P=0 for granite, 3.23 for clay and deep borehole, and 7.10 for salt)

This FEP is applicable to the host rock. The following processes are included:

- Saturated flow (flow sink)
- Unsaturated flow (capillary diversion, drift shadow)
- Influx/Seepage into EBS (film flow, enhanced seepage)

Because saturated conditions are assumed for all disposal concepts/geologic settings, only saturated flow related processes are applicable. Unsaturated conditions may exist in EDZ (to a lesser extent in the host rock) in case gas generation in EBS is significant. The effects on the host rock flow are closely related to the effects on the flow in EDZ, which are addressed in FEP 2.2.08.06, Flow through the EDZ.

For disposal in saturated units, excavations can provide preferred flow paths through the host rock or a groundwater sink. For these reasons, the effects of repository excavation are important for flow and transport, especially in low-permeability media, such as clay and salt. The preferential flow path is especially important for the Deep Borehole disposal concept because the borehole may create a direct path for flow and transport from the disposal zone to the shallower subsurface. Consequently, this FEP is important to clay, salt and borehole disposal concepts and is excluded for granite disposal concept based on low importance.

2.2.08.05 Condensation Forms in Host Rock (IS is not available, P=0)

This FEP is applicable only to host rocks. The following processes are included:

- Condensation cap
- Shedding

In water-saturated environments, condensation in the host rock is not likely to be a major process in the redistribution of water in host rock. Unsaturated conditions may exist in EDZ (to a lesser extent in the host rock) in case gas generation in EBS is significant. This FEP is excluded for all disposal concepts/geologic settings based on low consequences.

2.2.08.06 Flow through EDZ (IS=2.6, P=0 for granite, 3.65 for clay and deep borehole, and 7.73 for salt)

This FEP is applicable to EDZ. The following processes are included:

- Saturated / Unsaturated flow

- Fracture / Matrix flow

The EDZ properties are expected to be affected by fractures. The evolution of EDZ is described in FEP 2.01.01, Evolution of EDZ. The presence of fractures will enhance the permeability of the host rocks and will affect the flow in EDZ. However, the flow through the EDZ to a great extent will be controlled by the flow through the host rock. The flow through the host rocks is addressed in FEP 2.2.08.01, Flow through the Host Rock.

The host rock and other geologic units will control the travel times through the geosphere. Because of this flow through the EDZ is likely to be less important than flow through the host rock and other geologic units.

The only condition under which the flow through the EDZ might be of greater importance is when the EDZ provides for a complete flow circuit between the repository drifts and more permeable rock units outside the host rock. This may occur along excavations (including access excavations) or through the natural features, such as fractures or faults. . This process may have some importance for low-permeability media, such as clay and salt and for the Deep Borehole concept. Consequently, this FEP is considered important to clay, salt and borehole disposal concepts and is excluded for granite disposal concept based on low importance.

2.2.08.07 Mineralogic Dehydration (IS=1.2, P=0 for granite, 2.82 for clay and deep borehole, 6.49 for salt)

This FEP is applicable to all geosphere components. The following process is included:

- Dehydration reactions release water and may lead to volume changes.

Many minerals such as clay and zeolite contain water in the form of water molecule and/or hydroxyl. When the minerals are heated above their dehydration/dehydroxylation points they decompose into water and other minerals (typically denser phases). This process leads to release of water and volume change. As a result, the host rock strength, porosity and permeability may change. The changes in rock properties may affect the flow and transport through the rocks.

The magnitude of the impacts related to this FEP is a function of the type of hydrous minerals, their dehydration/dehydroxylation temperatures, their content in the rocks and the thermal profile. The changes will be negligible in the rocks located outside the thermal zone of influence from the repository.

Even in the thermally impacted zone, the effects are expected to be very small under the saturated conditions. This FEP is excluded for all geosphere components based on the low consequences.

2.2.08.08 Groundwater Discharge to Biosphere Boundary (IS is not available, P=0)

This FEP is applicable to all the geosphere components. However, it is most likely that the discharge to biosphere will occur from the other geologic units. The following processes are included:

- Surface discharge (water table, capillary rise, surface water)
- Flow across regulatory boundary

Groundwater discharge to the biosphere is controlled by the external flow boundary conditions. The main external flow boundary conditions are topography, sea level, surface water levels, regional inflow/outflow, and the amount and distribution of recharge. The recharge is addressed in Effects of Recharge on Geosphere Flow (FEP 2.2.08.03).

The boundary conditions may change due to a number of factors. Change in climate can result in changes to sea-level and surface water levels. The topography may change due to uplift and erosion. Human activities, such as dam construction, groundwater withdrawal, and agriculture, may have multiple impacts on the flow boundary conditions. These conditions are addressed in the External FEPs.

Groundwater from the other geologic units may discharge into the surface water bodies, unsaturated soils, and wetlands if any or all of these features are present. The discharge into these features will result in dilution of radionuclide concentrations. It is more conservative to assume that all the contaminated groundwater will be captured by a groundwater well.

Discharge to the biosphere is excluded for the host rock based on low consequence. Discharge to the biosphere is of some importance to the other geologic units.

Note that this FEP is not evaluated for its importance to the safety case in DOE (2011). This might be because the importance of this FEP is directly related to a regulatory framework, which has yet to be defined.

2.2.08.09 Groundwater Discharge to Well (IS is not available, P=0)

This FEP is applicable to all the geosphere components. However, it is most likely that the discharge to a well will occur from the other geologic units. The following processes are included:

- Human use (drinking water, bathing water, industrial)
- Agricultural use (irrigation, animal watering)

Discharge into a well is one of the most important pathways connecting radionuclide transport in geosphere and the biosphere. This is because the main exposure occurs via using contaminated groundwater.

The groundwater well is most likely to be located in an aquifer above the host rocks. Groundwater may also discharge into different surface water features and soils as discussed in FEP 2.2.08.08, Groundwater Discharge to Biosphere Boundary. However, it is more conservative to assume that a groundwater well will capture all the contaminant fluxes exiting from the host rock. This FEP is of high importance to the other geologic units and of low importance to the host rocks.

Note that this FEP is not evaluated for its importance to the safety case in DOE (2011). This might be because the importance of this FEP is directly related to a regulatory framework, which has yet to be defined.

2.2.09.01 Chemical Characteristics of Groundwater in Host Rock (IS=3, P=0 for granite, 2.4 for salt, 3.55 for clay, and 5.86 for deep borehole)

This FEP is applicable to host rocks and EDZ. The following processes are included:

- Water composition (radionuclides, dissolved species, …)
- Water chemistry (temperature, pH, Eh, ionic strength …)
- Reduction-oxidation potential
- Reaction kinetics
- Interaction with EBS
- Interaction with host rock

The chemical characteristics of water refer to the total concentrations of chemical constituents dissolved or suspended in the water and the aqueous species concentrations of dissolved constituents. These characteristics are affected by a number of factors, such as dilution, mixing, mineral dissolution, mineral precipitation, redox reactions, sorption, dissolution and exsolution of gases, and temperature.

The thermal effects on chemical characteristics are addressed in FEP 2.2.11.04, Thermal Effects on Chemistry and Microbial Activity in Geosphere. The changes of chemical characteristics in time are addressed in FEP 2.2.09.03, Chemical Interactions and Evolution of Groundwater in Host Rock. The chemical characteristics of water in EDZ are closely related to FEP2.1.09.01, Chemical Characteristics of Water Flowing into EBS.

Only a few radionuclides, such as inert gases and halides, are not affected by the composition of the water. The chemical characteristics have great impact on the transport of most of the radionuclides in both, EDZ and host rocks. This is because aqueous solubility limits and sorption might be highly sensitive to the chemical characteristics of the water. Decreased sorption may result in significantly faster (up to a few orders of magnitudes) transport times through the EDZ and host rocks.

The chemical characteristics of water in the EDZ may affect the corrosion and degradation rates in the EBS if this water flows into the EBS. The pH, temperature, and relative concentrations of chloride and nitrate can have a large effect on these rates, which, in turn, will affect the timing and rate of radionuclide releases from the waste packages.

This FEP has large impact on the radionuclide transport. All the processes included in this FEP are of high importance to the EDZ. All the processes included in this FEP, except interactions with the EBS, are of high importance to the host rocks. Interactions with the EBS are of some importance to the host rocks.

2.2.09.02 Chemical Characteristics of Groundwater in Other Geologic Units (IS=3, P=0 for granite, 2.4 for salt, 3.55 for clay, and 5.86 for deep borehole)

This FEP is applicable to the other geologic units. The following processes are included:

- Water composition (radionuclides, dissolved species, …)
- Water chemistry (temperature, pH, Eh, ionic strength …)
- Reduction-oxidation potential
- Reaction kinetics
- Interaction with other geologic units

The chemical characteristics of groundwater in the other geologic units have the same importance as the chemical characteristics of groundwater in the host rocks addressed in FEP 2.2.09.01, Chemical Characteristics of Groundwater in Host Rock. The chemical characteristics have significant impact on transport because they affect radionuclide aqueous solubility limits and sorption in the other geologic units.

The thermal effects on chemical characteristics are addressed in FEP 2.2.11.04, Thermal Effects on Chemistry and Microbial Activity in Geosphere. The changes of chemical characteristic in time are addressed in FEP 2.2.09.04, Chemical Interactions and Evolution of Groundwater in Other Geologic Units.

This FEP has large impact on the radionuclide transport. All the processes included in this FEP are of high importance to all the other geologic units.

2.2.09.03 Chemical Interactions and Evolution of Groundwater in Host Rock (IS=2, P=0 for granite, 2.1 for salt, 3.1 for clay, 5.4 for borehole)

This FEP is applicable to host rocks and EDZ. The following processes are included:

- 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
- Re-dissolution of precipitates after dry-out

This FEP considers the evolution of chemical composition of groundwater in host rocks and EDZ with time. The chemical evolution may affect the solubility and sorption characteristics, which, in turn, may affect radionuclide transport.

The evolution of groundwater chemistry might be affected by the presence of engineered materials in the EBS and heat from repository. Buffering of the minerals within the EDZ and host rocks is expected to prevent larger changes in groundwater composition along the entire flow path, except the buffering zone surrounding the EDZ and host rocks. The effects of chemical characteristics of groundwater in the EDZ and host rocks are addressed in FEP 2.2.09.01, Chemical Characteristics of Groundwater in Host Rock.

Waste heat may change equilibrium conditions and increase reaction rates. However, the thermal period is expected to be short compared to the regulatory period and the thermal zone of influence is expected to be of a limited extent. The thermal effects on chemical characteristics are also addressed in FEP 2.2.11.04, Thermal Effects on Chemistry and Microbial Activity in Geosphere.

Natural changes in water composition may occur due to changes in recharge water chemistry caused by new sources or types of recharge and climate change. Alternatively, natural changes may result from changes in system conditions, such as temperature and pressure. Such changes could be caused by uplift or changes in regional stress. Additional natural changes in composition are possible if changes in igneous or geothermal processes affect the system. These changes are considered under the External FEPs.

The changes in groundwater compositions require very long time to occur. Groundwater composition in the geosphere is generally in near steady state with respect to minerals along the flow path. This steady state is expected to continue far into the future.

This FEP is included for all disposal concepts/geologic setting as somewhat important to EDZ and host rock mainly to account for interactions with EBS.

Note that this FEP has medium importance score in DOE (2011). This might be attributed to the high importance of the chemical composition of the host rock in general, which is addressed in FEP 2.2.09.01, Chemical Characteristics of Groundwater in Host Rock. The arguments provided above suggest that the changes in chemical composition in time (or evolution) will be small.

2.2.09.04 Chemical Interactions and Evolution of Groundwater in Other Geologic Units (IS=2, P=0 for granite, 2.1 for salt, 3.1 for clay, 5.4 for borehole)

This FEP is applicable to the other geologic units. The following processes are included:

- Other geologic unit composition and evolution (granite, clay, salt ...)
- Evolution of water chemistry in other geologic units
- Chemical effects on density
- Interaction with EBS
- Reaction kinetics
- Mineral dissolution/precipitation
- Re-dissolution of precipitates after dry-out

This FEP considers the evolution of chemical composition of groundwater in the other geologic units with time. The engineered materials in the EBS and the repository heat are expected to have a very small impact on the other geologic units because of the large distance between the repository and the other geologic units.

The evolution of chemical composition in the other geologic units may occur due to natural causes, which are the same as in the case of EDZ and host rocks (FEP 2.2.09.03, Chemical Interactions and Evolution of Groundwater in Host Rock).

Groundwater composition in the other geologic units is likely to be near steady state with respect to minerals along the flow path. There might be some trends in water composition related to its age. However, the sharp temporal changes indicative of a major change in groundwater composition at some point in time are unlikely.

This FEP is excluded for all the other geologic units based on the low consequences.

Note that this FEP has medium importance score in DOE (2011). This might be attributed to the high importance of the chemical composition of the other geologic units in general, which is addressed in FEP 2.2.09.02, Chemical Characteristics of Groundwater in Other Geologic Units. The arguments provided above suggest that the changes in chemical composition in time (or evolution) will be small.

2.2.09.05 Radionuclide Speciation and Solubility in Host Rock (IS=3, P=0 for granite, 2.4 for salt, 3.55 for clay, and 5.86 for deep borehole)

This FEP is applicable to host rocks and EDZ. The following process is included:

- Dissolved concentration limits

Maximum concentrations of radionuclides in the host rock and EDZ are limited by the concentrations of radionuclides released from EBS. If the radionuclide solubilities in the EDZ and host rocks are higher than in EBS, there will be no impacts on radionuclide transport. Radionuclide transport may be affected if the chemical conditions in the host rock and EDZ, such as pH, redox conditions, mineral equilibrium, will decrease radionuclide solubilities below the concentrations released from the EBS. In this case, the radionuclide concentrations will be reduced to match the new solubility limits. This is true as long as the primary chemical conditions in the host rock that control radionuclide solubility do not change significantly over time. Evolution of chemical properties is addressed in FEP 2.2.09.03, Chemical Interactions and Evolution of Groundwater in Host Rock. The exception includes solubility-limited radionuclide daughters generated in the host rock and/or EDZ.

The transport of many radionuclides through the host rock and EDZ will not be constrained or affected by speciation or solubility. This FEP is excluded for all disposal concepts/geologic settings based on the low consequences.

Note that this FEP has high importance score in DOE (2011). This might be attributed to the high importance of this FEP for EBS. However, as discussed above, the dissolved concentration limits do not enhance radionuclide transport in EDZ and host rock and thus have low importance in this evaluation.

2.2.09.06 Radionuclide Speciation and Solubility in Other Geologic Units (IS=3, P=0 for granite, 2.4 for salt, 3.55 for clay, and 5.86 for deep borehole)

This FEP is applicable to the other geologic units. The following process is included:

- Dissolved concentration limits

Same considerations as described in FEP 2.2.09.05, Radionuclide Speciation and Solubility in Host Rock, are applicable to radionuclide speciation and solubility in the other geologic units.

The transport of many radionuclides through the other geologic units will not be constrained or affected by speciation or solubility. This FEP is excluded for all the other geologic units based on the low consequences.

Note that this FEP has high importance score in DOE (2011). This might be attributed to the high importance of this FEP for EBS. However, as discussed above, the dissolved concentration limits do not enhance radionuclide transport in other geologic units and thus have low importance in this evaluation.

2.2.09.51 Advection of Dissolved Radionuclides in Host Rock (IS=2.8, P=2.53 for salt and deep borehole, and 3.74 for clay and granite)

This FEP is applicable to host rocks. The following processes are included:

- Flow pathways and velocity
- Advective properties (porosity, tortuosity)
- Dispersion
- Matrix diffusion
- Saturation

Advection of dissolved radionuclides through the host rock is closely related to the FEP 2.2.08.01, Flow through the Host Rock. The principal differences in these FEPs are the differences between the flow rate and transport velocity. The transport velocity is a function of flow rate and porosity. In addition to this, it may be affected by matrix diffusion, dispersion, sorption, complexation and presence of colloids. Sorption is addressed in FEP 2.2.09.55, Sorption of Dissolved Radionuclides in Host Rock. Diffusion is addressed in FEP 2.2.09.53, Diffusion of Dissolved Radionuclides in Host Rock. Complexation is addressed in FEP 2.2.09.57,Complexation in Host Rock. Effects of colloids on the advective transport are addressed in FEP2.2.09.59, Colloidal Transport in Host Rock.

Under saturated repository conditions, the advective flow through the host rock is one of the most important pathways affecting radionuclide transport in geosphere. Radionuclide transport by advective flow, or radionuclide advection, is highly important for Granite and Deep Borehole disposal concepts because the advective flow is a dominant transport mechanism in the fractured media.

In the low-permeability media, such as clay and shale, advective flow may still be important (this depends on site-specific conditions) as discussed under FEP 2.2.08.01. Advective transport has low probability in salt.

Based on the impacts on radionuclide transport, advection is assigned high importance for Granite and Deep Borehole concepts, some importance for Clay concept, and low importance for Salt concepts.

2.2.09.5 Advection of Dissolved Radionuclides in Other Geologic Units (IS=2.8, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to the other geologic units. The following processes are included:

- Flow pathways and velocity
- Advective properties (porosity, tortuosity)
- Dispersion
- Matrix diffusion
- Saturation

Advection of dissolved radionuclides through the other geologic units is closely related to the FEP 2.2.08.02, Flow through the Other Geologic Units. The principal differences in these FEPs are the differences between the flow rate and transport velocity.

The transport velocity is a function of flow rates and porosities in the other geologic units. In addition to this, it may be affected by matrix diffusion, dispersion, sorption, complexation and presence of colloids. Sorption is addressed in FEP 2.2.09.56, Sorption of Dissolved Radionuclides in Other Geologic Units. Diffusion is addressed in FEP 2.2.09.54, Diffusion of Dissolved Radionuclides in Other Geologic Units. Complexation is addressed in FEP 2.2.09.58,Complexation in Other Geologic Units. Effects of colloids on advective transport are addressed in FEP 2.2.09.60, Colloidal Transport in Other Geologic Units.

Flow through the other geologic units is the most important pathway through which the radionuclides released from the host rocks are transported to biosphere. The flow in an aquifer is especially important because it affects the radionuclide concentrations in the groundwater well that directly affects the exposure doses. Consequently, radionuclide transport by advective flow in an aquifer has very high importance. Because the advective flow may be small in low-permeability media, such as confining units, radionuclide advection may or may not be important depending on the site-specific conditions in these units.

Radionuclide advection in the other geologic units is of high importance to the aquifer and of some importance to the confining units.

2.2.09.53 Diffusion of Dissolved Radionuclides in Host Rock (IS=3, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to host rocks. The following processes are included:

- Gradients (concentration, chemical potential)
- Diffusive properties (diffusion coefficients)
- Flow pathways and velocity
- Saturation

Diffusion of dissolved radionuclides through the host rock is an alternative transport mechanism to advection. Diffusion is especially important in the low-permeability host rocks, such as clay/shale and salt. In these rocks, diffusion may be either dominant or comparable (except salt) with advective transport, depending on the transport distances and rock properties as discussed in FEP 2.2.08.01, Flow through the Host Rock. Diffusion is likely to be of low importance to radionuclide transport in fractured hard rocks where advection is, by far, a dominant mechanism.

The diffusion flux is a function of concentration gradient and effective diffusion coefficient. The effective diffusion coefficient is affected by the porosity of the host rocks and by the radionuclide-specific parameters, such anion exclusion and sorption. Because clay and shale have very small pore spaces, electrochemical interactions (ion exclusion) can affect pore accessibility differently for different solutes. Sorption is addressed in FEP 2.2.09.55, Sorption of Dissolved Radionuclides in Host Rock.

The diffusion coefficient is temperature-dependent, increasing with increasing temperature. Temperature dependence is understood theoretically based on the Stokes-Einstein equation. Thermal diffusion is addressed in FEP 2.2.11.05, Thermal Effects on Transport in Geosphere.

Diffusion coefficients have been found to be correlated with porosity and permeability in tuff matrix (Reimus et al. 2007). Diffusion coefficients measured in clay and shale showed difference in magnitude for diffusion parallel or perpendicular to bedding (Mazurek et al. 2003, p. 121).

For high radionuclide solution concentrations, the effective diffusion coefficient can show concentration dependence.

Based on the impacts on radionuclide transport, diffusion is assigned high importance for Clay and Salt concepts and some importance for Granite and Deep Borehole concepts.

2.2.09.54 Diffusion of Dissolved Radionuclides in Other Geologic Units (IS=3, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to the other geologic units. The following processes are included:

- Gradients (concentration, chemical potential)
- Diffusive properties (diffusion coefficients)
- Flow pathways and velocity
- Saturation

Diffusion of dissolved radionuclides in the other geologic units might be an important transport mechanism in case of confining units. The same considerations apply to diffusion in confining units as the ones for shale/clay and salt discussed in FEP 2.2.09.53. Diffusion is likely to be of low importance to the radionuclide transport in the aquifers where advection is a dominant transport mechanism.

Based on the impacts on radionuclide transport, the diffusion is assigned high importance for confining units and some importance for aquifers.

2.2.09.55 Sorption of Dissolved Radionuclides in Host Rock (IS=3, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to host rocks. The following processes are included:

- Surface complexation properties
- Flow pathways and velocity
- Saturation

Sorption includes covalent bonding, ionic bonding, and diffuse double-layer attraction to immobile geologic media. It also includes partitioning to, and complexation with, immobile organic matter.

Sorption in host rocks interacts with two major radionuclide transport mechanisms, advection and diffusion, and because of this is one of the most important processes. Sorption impacts transport by changing the effective advective and diffusive transport velocities.

Sorption of dissolved and colloidal radionuclides can occur on the surfaces of both fractures and matrix in rock along the transport path. Sorption to colloids is considered in FEP 2.2.09.59, Colloidal Transport in Host Rock.

Sorption may be reversible or irreversible, and it may occur as a linear or nonlinear process. Sorption kinetics and the availability of sites for sorption need to be considered when selecting an appropriate sorption model. Sorption is radionuclide specific and is a function of mineral type and groundwater composition. Sorption may also be temperature dependent.

Sorption in fractures might be less significant than in rock matrix because of the low surface area to volume for fractures as compared with rock matrix.

Due to its significant effects on major transport mechanisms, sorption is assigned high importance to all disposal concepts/geologic settings.

2.2.09.56 Sorption of Dissolved Radionuclides in Other Geologic Units (IS=3, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to the other geologic units. The following processes are included:

- Surface complexation properties
- Flow pathways and velocity
- Saturation

Sorption in the other geologic units interacts with two major radionuclide transport mechanisms, advection and diffusion, and because of this is one of the most important processes.

The same considerations as the ones related to the sorption in the host rocks discussed in FEP 2.2.09.55 apply to the sorption in the other geologic units. Sorption to colloids is considered in FEP 2.2.09.60, Colloidal Transport in Other geologic Units.

Due to its significant effects on major transport mechanisms, sorption in confining units and aquifers is assigned high importance. Sorption in the unsaturated zone above the aquifer is of lower importance because the major flow and transport pathways occur in the saturated zone.

2.2.09.57 Complexation in Host Rock (IS=3, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to both, host rocks and EDZ. The following processes are included:

- Presence of organic complexants (humates, fulvates, carbonates, …)

- Enhanced transport of radionuclides associated with organic complexants

Complexing agents such as carbonate, fluoride, and humic and fulvic acids present in natural groundwater may affect radionuclide transport in the EDZ and host rocks. The organic complexant may be also introduced into the groundwater in EDZ and host rocks from the engineered materials used in EBS. This FEP considers complexation with dissolved organic compounds and organic matter. Complexation with immobile organic matter is considered in FEP 2.2.09.55, Sorption of Dissolved Radionuclides in Host Rock.

Inorganic and organic complexing agents may mobilize high and moderately sorbing radionuclides if they form strong low sorbing complexes with these radionuclides. Complexing agents may also affect speciation of radionuclides in groundwater, and as a consequence, affect their sorption onto the rock surface and colloids.

Complexation may increase the solubility of the radionuclide in the EDZ and host rocks. This is important in the case when the radionuclide solubilities in the EDZ and host rocks are lower than radionuclide concentrations released from the EBS.

Transport may also be enhanced by complexation with colloidal dissolved organic matter such as fulvic and humic acids. Colloidal transport is addressed in FEPs 2.2.09.59, Colloidal Transport in Host Rock.

Complexation may be of high importance for some radionuclides if the compexants in the groundwater are available. Otherwise, complexation may have low importance. In the absence of site-specific data, complexation is considered to be somewhat important for all disposal concepts/geologic settings.

2.2.09.58Complexation in Other Geologic Units (IS=3, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to the other geologic units. The following processes are included:

- Presence of organic complexants (humates, fulvates, carbonates, …)
- Enhanced transport of radionuclides associated with organic complexants

Complexing agents such as carbonate, fluoride, and humic and fulvic acids present in natural groundwater may affect radionuclide transport in the other geologic units. This FEP considers complexation with dissolved organic compounds and organic matter. Complexation with immobile organic matter is considered in FEP 2.2.09.56, Sorption of Dissolved Radionuclides in Other Geologic Units.

The same considerations as the ones for the EDZ and host rocks discussed in FEP 2.2.09.57 apply to the complexation in the other geologic units. The only difference is in the complexant availability. The groundwater in shallow aquifers is likely to have more organic complexants.

Complexation may be of high importance for some radionuclides if the compexants in the groundwater are available. Otherwise, complexation may have low importance. In the absence of site-specific data, complexation is considered to be somewhat important for all the components of the other geologic units.

2.2.09.59 Colloidal Transport in Host Rock (IS=2.38, P=2.22 for salt and deep borehole, and 3.29 for clay and granite)

This FEP is applicable to both, host rocks and EDZ. The following processes are included:

- Flow pathways and velocity
- Saturation
- Advection
- Dispersion
- Diffusion
- Sorption
- Colloid concentration

Colloids in the EDZ and host rocks include intrinsic colloids (colloidal size radionuclide polymers/particles), waste form colloids, and pseudocolloids (non-radioactive colloids, such as mineral fragments, microbes, microbe fragments, and humic and fulvic acids with sorbed radionuclides).

Processes include formation and stability of these colloids, sorption of radionuclides on these colloids, and colloidal transport processes. Transport of colloids, as well as transport of radionuclides, includes advection, dispersion, and diffusion. Transport of colloids, as well as transport of radionuclides, is affected by sorption and pore-size exclusion. Transport of colloids is important because some radionuclides may attach to colloids. This provides an additional mechanism of radionuclides transport.

The same advection, diffusion, and sorption considerations as for the dissolved radionuclides apply to colloids. These considerations are discussed in the following FEPs: FEP 2.2.09.51, Advection of Dissolved Radionuclides in Host Rock; FEP 2.2.09.53, Diffusion of Dissolved Radionuclides in Host Rock; and FEP 2.2.09.55, Sorption of Dissolved Radionuclides in Host Rock.

Colloids may increase or decrease the transport of a particular radionuclide. It may increase it by increasing the mobility of the radionuclide. This is especially important for radionuclides with low solubility and/or high sorption. Colloids may also facilitate transport because they may be physically excluded from small pores where ground water velocities are lower. Alternatively, colloids may sorb or become immobilized by filtration. Sorption of colloids may be less effective in fracture media because of the low surface area to volume for fractures as compared with rock matrix.

The effect of colloids on radionuclide transport is highly specific to the particular radionuclide, the type of colloid, and the properties of the EDZ and host rocks. Colloidal transport may be of high importance for some radionuclides if the colloids in the groundwater are present in sufficient concentrations. Otherwise, the colloidal transport may have low importance. In the absence of site-specific data, the colloidal transport is considered to be somewhat important for all disposal concepts/geologic settings.

2.2.09.60 Colloidal Transport in Other Geologic Units (IS=2.38, P=2.22 for salt and deep borehole, and 3.29 for clay and granite)

This FEP is applicable to the other geologic units. The following processes are included:

- Flow pathways and velocity
- Saturation
- Advection
- Dispersion
- Diffusion
- Sorption
- Colloid concentration

Colloidal transport in the other geologic units includes formation and stability of colloids, sorption of radionuclides on colloids, and colloidal transport via advection, dispersion, and diffusion. The same advection, diffusion, and sorption considerations as for the dissolved radionuclides apply to colloids. These considerations are discussed in the following FEPs: FEP 2.2.09.52, Advection of Dissolved Radionuclides in Other Geologic Units; FEP 2.2.09.54, Diffusion of Dissolved Radionuclides in Other Geologic Units; and FEP 2.2.09.56, Sorption of Dissolved Radionuclides in Other Geologic Units.

The same considerations as the ones for the EDZ and host rocks discussed in FEP 2.2.09.59 apply to the colloidal transport in the other geologic units. The effect of colloids on radionuclide transport is highly specific to the particular radionuclide, the type of colloid, and the properties of the other geologic units. Colloidal transport may be of high importance for some radionuclides if the colloids in the groundwater are present in sufficient concentrations. Otherwise, the colloidal transport may have low importance. In the absence of site-specific data, colloidal transport is considered to be somewhat important for the confining units and aquifers. Colloidal transport is of low importance to the unsaturated zone because the major flow and transport pathways are in the saturated zone aquifer and confining units.

2.2.09.61 Radionuclide Transport Through EDZ (IS=3, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to both, host rocks and EDZ. The following processes are included:

- Advection
- Dispersion
- Diffusion
- Sorption

This FEP is closely related to the following FEPs: FEP 2.2.08.06, Flow through EDZ; FEP 2.2.09.51, Advection of Dissolved Radionuclides in Host Rock; FEP 2.2.09.53, Diffusion of Dissolved Radionuclides in Host Rock; and FEP 2.2.09.55, Sorption of Dissolved Radionuclides in Host Rock.

Flow and transport processes in the EDZ are the same as in the host rocks, but the flow and transport properties might be different. The primary differences between the EDZ and host rock are due to the repository excavation, waste heat, and presence of engineered materials in EBS. Excavation activities may cause fractures and fractures may enhance the permeability of the EDZ, expose mineral surfaces to weathering processes, provide new surfaces for sorption, and potentially generate colloids. Heat from repository may affect the diffusion coefficients and sorption.

The presence of engineered materials will impact the chemical composition of the groundwater in the EDZ, which, in turn, will impact sorption. The EDZ is also distinguished chemically because of the oxidation of minerals during excavation and pre-closure operations as well as exposure to generally higher temperatures.

Because the EDZ size is expected to be small compared to the spatial dimensions of the host rock, configuration of EDZ and other natural flow pathways, the processes related to this FEP should have moderate importance for all disposal concepts/geologic settings.

High importance of this FEP for transport may be expected when a complete flow circuit between the repository drifts and more permeable rock units outside the host rock could result in much stronger advective radionuclide transport out of the host rock. This situation has higher probability in the case of the Deep Borehole disposal concept.

2.2.09.62 Dilution of Radionuclides in Groundwater (IS=2, P=2.1 for salt and deep borehole, and 3.1 for clay and granite)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Mixing with uncontaminated groundwater
- Mixing at withdrawal well

This FEP is closely related to FEP 2.2.08.08, Groundwater Discharge to Biosphere Boundary,and FEP 2.2.08.09, Groundwater Discharge to Well.

This FEP is applicable to all geosphere components. However, it is most likely that mixing with uncontaminated groundwater will occur in an aquifer. Also, the groundwater well is most likely to be located in an aquifer above the host rocks.

Significant dilution can occur at a groundwater well that captures both contaminated and uncontaminated groundwater. Significant dilution can also occur in case when an aquifer receives significant recharge or in case when contaminated groundwater discharges into a surface water body.

Although dilution does not necessarily reduce the amount of radioactivity that reaches the biosphere, it does reduce the concentrations at the exposure points. The mixing with uncontaminated groundwater and mixing at the withdrawal well will have significant impacts on the radionuclide concentrations in the well water, which is the major exposure pathway.

This FEP has high importance for aquifers and low importance for the other geologic units, host rocks, and EDZ.

2.2.09.63 Dilution of Radionuclides with Stable Isotopes (IS=2, P=2.1 for salt and deep borehole, and 3.1 for clay and granite)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following process is included:

- Mixing with stable and/or naturally occurring isotopes of the same element

Mixing of radionuclide isotopes from the repository waste with the naturally occurring stable isotopes of the same element in groundwater may occur for some radionuclides, resulting in a lower effective dose. This primarily concerns ^{129}I mixing with stable ^{127}I; ^{36}Cl mixing with stable ^{35}Cl and ^{37}Cl; and ^{90}Sr mixing with stable ^{84}Sr,^{86}Sr, ^{87}Sr, and ^{88}Sr.

Chemical and physical processes that result in competition among radioactive and stable isotopes may lead to an isotopic dilution effect. The magnitude of the effect of isotopic dilution depends on the relative amounts of the radioactive and corresponding stable isotopes of the same element, as well as the competitive effects on retention for that element in the human body and corresponding radiological dose.

It is expected that the concentrations of the naturally occurring stable isotopes of the radionuclides contained in the wastes will be low and the consequences of the isotopic dilution will be negligible. Many other radionuclides, such as isotopes of technetium, plutonium, and americium contained in the wastes are rare in the natural environment and isotopic dilution would not occur.

This FEP is excluded from all disposal concepts/geologic settings and all components of the other geologic units based on low consequences.

Note that this FEP has medium importance score in DOE (2011). This acknowledges the fact that mixing of radionuclide isotopes from the waste with the naturally occurring stable isotopes of the same element in groundwater may occur for some radionuclides. However, as discussed above, this process results in lower concentrations. Consequently, this FEP has low importance in this evaluation.

2.2.09.64Radionuclide Release from Host Rock (IS=3, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to host rocks. The following process is included:

- Spatial and temporal distribution of releases to the Other Geologic Units or to the Biosphere (due to varying flow pathways and velocities, varying transport properties)

This FEP is closely related to FEP 2.2.08.08, Groundwater Discharge to Biosphere Boundary, and FEP 2.2.08.09, Groundwater Discharge to Well.

The spatial and temporal distribution of radionuclide releases from the host rocks to the other geologic units has significant impact on the radionuclide concentrations in the other geologic units, which, in turn, impact the radionuclide concentrations at the exposure points and the corresponding exposure doses. Spatial distribution is controlled by the flow and transport pathways through the host rocks. Temporal distribution is controlled by the temporal distribution of the releases from the EBS and by the transport processes in the host rocks. Flow and transport in the host rocks are considered in FEPs 2.2.09.51; 2.2.09.53; 2.2.09.55; 2.2.09.57; and 2.2.09.59.

This FEP is of high importance to all disposal concepts/geologic settings due to its significant consequences for the exposure doses.

2.2.09.65 Radionuclide Release from Other Geologic Units (IS=3, P=2.4 for salt and deep borehole, and 3.55 for clay and granite)

This FEP is applicable to the other geologic units. The following process is included:

- Spatial and temporal distribution of releases to the Biosphere (due to varying flow pathways and velocities, varying transport properties)

This FEP is closely related to FEP 2.2.08.08, Groundwater Discharge to Biosphere Boundary, and FEP 2.2.08.09, Groundwater Discharge to Well.

The spatial and temporal distribution of radionuclide releases from the other geologic units to the biosphere has significant impact on the radionuclide concentrations at the exposure points and the corresponding exposure doses. Spatial distribution is controlled by the flow and transport pathways through the other geologic units. Temporal distribution is controlled by the temporal distribution of the releases from the host rocks and by the transport processes in the other geologic units. The flow and transport in the other geologic units are considered in FEPs 2.2.09.52; 2.2.09.54; 2.2.09.56; 2.2.09.58; and 2.2.09.60.

This FEP is of high importance to all the components of the other geologic units due to its significant consequences for the exposure doses.

2.2.10.01 Microbial Activity in Host Rock (IS=2, P=1.32)

This FEP is applicable to host rocks. The following processes are included:

- Formation of complexants
- Formation and stability of microbial colloids
- Biodegradation
- Bioaccumulation

Microbial activity in the host rocks may affect radionuclide transport and supply of corrosive reactants.

Microbial activity in the host rock can affect radionuclide transport via formation of complexants and microbial colloids, biodegradation, and bioaccumulation. Microbial activity in the host rock may also affect the supply of corrosive reactants, such as hydrogen sulfide and organic acid that enter the EBS. Hydrogen sulfide, a corrosive reactant to a copper canister, is produced by sulfate-reducing bacteria, which are commonly found at depth.

The factors that affect underground microbial activity are environmental (such as temperature) and supply of nutrients (such as oxygen, organic carbon, nitrate, and phosphate). These factors will vary widely depending on the specific location and repository design even within a given generic disposal concept. However, the nutrient supply deep in the geosphere will most likely be insufficient to produce any significant consequences.

This FEP is excluded from all disposal concepts/geologic settings based on low consequences.

Note that this FEP has medium importance score in DOE (2011). This acknowledges the fact that microbial activity in the host rock may affect radionuclide transport via formation of complexants and microbial colloids, biodegradation, and bioaccumulation. However, as discussed above, the extent of these processes are likely to be very limited in the environments common for the host rocks. Consequently, this FEP has low importance in this evaluation.

2.2.10.02 Microbial Activity in Other Geologic Units (IS=2, P=1.32)

This FEP is applicable to the other geologic units. The following processes are included:

- Formation of complexants
- Formation and stability of microbial colloids
- Biodegradation
- Bioaccumulation

Microbial activity in the other geologic units can affect radionuclide transport via formation of complexants and microbial colloids, biodegradation, and bioaccumulation. The microbial activity is most likely to take place in soils in the unsaturated zone, where the nutrients are abundant. In this case, the radionuclides associated with microbes can potentially bioaccumulate in higher organisms in a food chain and cause higher exposure doses. However, the major transport pathways are located within the saturated zone where microbial activity is limited.

This FEP is excluded from all components of the other geologic units based on low consequences.

Note that this FEP has medium importance score in DOE (2011). This acknowledges the fact that microbial activity in the other geologic units may affect radionuclide transport via formation of complexants and microbial colloids, biodegradation, and bioaccumulation. However, as discussed above, the extent of these processes are likely to be very limited along the major transport pathway (saturated zone). Consequently, this FEP has low importance in this evaluation.

2.2.11.01 Thermal Effects on Flow in Geosphere (IS=2, P= 2.1 for granite and salt and 3.1 for clay and deep borehole)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Altered saturation / relative humidity (dry-out, re-saturation)
- Altered gradients, density, and/or flow pathways
- Vapor flow
- Condensation

This FEP is closely related to the following FEPs: FEP 2.2.08.01, Flow through the Host Rock, FEP 2.2.08.02, Flow through Other Geologic Units, FEP 2.2.08.06, Flow through EDZ, and FEP 2.2.05.03, Alteration and Evolution of Geosphere Flow Pathways.

Under saturated repository conditions altered saturation, relative humidity, vapor flow, and condensation have low consequences. Unsaturated conditions may occur in the EDZ in the case of significant gas generation in the EBS.

Two significant thermal effects on flow due to the heat from repository might be reduction in viscosity and density of groundwater. The reduction in density has two effects: (1) an initial outflow during heat-up resulting from thermal expansion of the water and, a flow back toward the heat source as temperatures return to ambient (2) buoyant convection driven by the reduced density of the heated water.

The first process is expected to have low consequences. It is anticipated that Granite, Clay, and Salt repository designs will have thermal limits on the peak waste package temperature. Maintaining these peak temperatures below the corresponding limits will result in moderate impact on the temperatures of the host rocks and especially other geologic units and relatively short (compared to the regulatory period) time of thermal period. The temperature limits are not applicable to the Deep Borehole. However, the zone of influence from the borehole will be significantly smaller than zone of influence from a repository.

Convection is considered in FEP 2.2.11.02, Thermally-Driven Flow (Convection) in Geosphere.

All the processes in this FEP are considered to be of low significance for all the disposal concepts/geologic settings and for all the components of the other geologic units, except convection (altered gradients, density, and/or flow pathways). Convection is of some importance to Granite and Deep Borehole disposal concepts.

2.2.11.02 Thermally-Driven Flow (Convection) in Geosphere (IS=2, P= 2.1 for granite and salt and 3.1 for clay and deep borehole)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Convection

Repository heating will lead to reduced densities of the groundwater within the zone of thermal influence during the thermal period. Lower density will cause the higher temperature groundwater to rise due to buoyancy until temperature equilibrium is achieved.

Convection has low consequences in the other geologic units because most likely the temperature changes will be small due to the large distances from these units to the repository.

Convection will probably be week in clay/shale and salt host rocks due to relatively low density gradients and low permeability. Convection in granite rocks may be of higher importance, especially if the fracture network is sub-vertical.

The other possible cause of buoyancy-driven flow is the introduction of some other natural geo-fluid such as CO_2, hydrocarbons, or geothermally heated water. Of these, geothermal water has the greatest potential to affect radionuclide transport because of misciblity with the formation water. However, the probability of geothermal intrusion is low.

This FEP is of some importance to Granite and Deep Borehole disposal concepts. This FEP is excluded for the Clay/Shale and Salt disposal concepts and for all the components of the other geologic units based on low consequences.

2.2.11.03 Thermally-Driven Buoyant Flow / Heat Pipes in Geosphere (IS=1, P= 1.6 for granite and salt and 2.46 for clay and deep borehole)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following process is included:

- Vapor flow

Under the saturated repository conditions vapor flow and potential development of heat pipes has low consequences. Unsaturated conditions may occur in the EDZ in the case of significant gas generation in the EBS.

This FEP is excluded from all disposal concepts/geologic settings and all the components of the other geologic units based on low consequences.

2.2.11.04 Thermal Effects on Chemistry and Microbial Activity in Geosphere (IS=3, P= 2.4 for granite and salt and 3.55 for clay and deep borehole)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Mineral precipitation / dissolution
- Altered solubility

Thermal effects may affect radionuclide transport directly by causing changes in radionuclide speciation and solubility or, indirectly, by causing changes to host rock mineralogy that affect the flow paths.

Radionuclide solubility and speciation are addressed in FEP 2.2.09.05, Radionuclide Speciation and Solubility in Host Rock and FEP 2.2.09.06, Radionuclide Speciation and Solubility in Other Geologic Units. The effects of solubility and speciation are evaluated to be of low importance in these FEPs.

Precipitation and dissolution may have some impact on the granite rocks because fracture permeability may change as a result of mineral precipitation (fracture filling) or dissolution.

However, these processes will be limited to the zone of thermal influence. The reaction may reverse when the thermal period ends.

This FEP is excluded from all disposal concepts/geologic settings and all the components of the other geologic units based on low consequences.

2.2.11.05 Thermal Effects on Transport in Geosphere (IS is not available, P=0)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Thermal diffusion (Soret effect)
- Thermal osmosis

In most aqueous solutions, ions diffuse preferentially in the direction of the thermal gradient. This effect depends mainly on the magnitude of the Soret coefficient and the temperature gradient. The effects on diffusion may only be important for the low-permeability rocks in which diffusional transport is an important mechanism.

The Soret coefficients at steady state are in the order of 10^{-3} to 10^{-2} 1/K depending on the type of solution (Platten, 2006). The thermal diffusion coefficient is then 10^{-3} to $10^{-2}$of the chemical diffusion coefficient (Fickian transport). Consequently, in case of a moderate temperature gradient the role of thermal diffusion is small.

This FEP is excluded from all disposal concepts/geologic settings and all the components of the other geologic units based on low consequences.

2.2.11.06 Thermal-Mechanical Effects on Geosphere (IS=2.38, P= 2.3 for granite and salt and 3.4 for clay and deep borehole, likely to be screened out in far field)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Thermal expansion / compression
- Altered properties of fractures, faults, rock matrix

Heat from the waste causes thermal expansion of the surrounding rock, generating changes in the stress field that may change the properties (both hydrologic and mechanical) of fractures in the rock and generate new fractures. Cooling following the peak thermal period will also change the stress field, further affecting fracture properties near the repository.

The mechanical effects are also addressed in FEP 2.2.07.01, Mechanical Effects on Host Rock and FEP 2.2.07.02 Mechanical Effects on Other Geologic Units.

It is expected that the mechanical effects will be small due to the relatively small size of the zone of thermal influence and due to short duration of the thermal period compared to the regulatory period.

This FEP has some importance for Deep Borehole disposal concept. It is excluded for all the other disposal concepts/geologic setting and all the components of the other geologic units.

2.2.11.07 Thermal-Chemical Alteration of Geosphere (IS=2.38, P= 2.3 for granite and salt and 3.4 for clay and deep borehole, likely to be screened out in far field)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Mineral precipitation / dissolution
- Altered properties of fractures, faults, rock matrix
- Alteration of minerals / volume changes
- Formation of near-field chemically altered zone (rind)

Thermal-chemical alteration due to mineral precipitation and dissolution is addressed in FEP 2.2.11.04, Thermal Effects on Chemistry and Microbial Activity in Geosphere. The formation of a near-field chemically altered zone has similar effects as precipitation. Alteration of minerals and volume changes are addressed in FEP 2.2.08.07, Mineralogic Dehydration.

Altered properties of fractures are considered in FEP 2.2.11.05, Thermal Effects on Transport in Geosphere. The effects on the faults and rock matrix are similar to the ones identified for fractures.

This FEP is excluded from all disposal concepts/geologic settings and all the components of the other geologic units based on low consequences.

2.2.12.01 Gas Generation in Geosphere (IS is not available, P=0)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Degassing (clathrates, deep gases)
- Microbial degradation of organics
- Vaporization of water

Potential gas sources include degradation of repository components and naturally occurring gases from clathrates, microbial degradation of organic material, and deep gases from hydrocarbons from a nearby formation containing natural gas.

Pressure variations due to gas generation may affect flow patterns and contaminant transport in the geosphere. The generation of gas can affect radionuclide transport by producing gas bubbles and gas phase. Degassing may affect flow and transport of gaseous contaminants.

Vaporization of water has low consequences under saturated repository conditions, moderate temperature increase outside of EBS, and short duration of thermal period compared to the regulatory period.

Microbial degradation of organics is considered in FEP 2.2.10.01, Microbial Activity in Host Rock and FEP 2.2.10.02, Microbial Activity in Other Geologic Units. The microbial activity in host rocks is expected to be limited due to insufficient nutrient supply deep in the geosphere. Nutrient supply might be more abundant in the other geologic units, such as unsaturated zone and soils. However, the major transport pathways are located within the saturated zone where microbial activity is limited. As a result, gas generation due to microbial activities in both host rocks and other geologic units will have low consequences.

Degassing may occur due to pressure and temperature changes in geosphere. As a result, nitrogen or carbon dioxide might exsolve from water and methane might exsolve from clathrates. However, the expected changes in pressures and temperatures are not large enough to produce any significant amounts of gas.

This FEP is excluded from all disposal concepts/geologic settings and all the components of the other geologic units based on low consequences.

2.2.12.02 Effects of Gas on Flow through the Geosphere (IS=2, P=0.95, likely to be screened out)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Altered gradients and/or flow pathways
- Vapor/air flow
- Two-phase flow
- Gas bubbles

This FEP addresses effects resulting from the presence of a gas phase in the geosphere. This FEP is closely related to FEP 2.2.12.01, Gas Generation in Geosphere. Gas bubbles and gas phase may alter aqueous flow pathways, trap volatile, semi-volatile, or colloidal radionuclides, or transport radionuclides in the gas phase.

Vapor/air and two-phase flow have low consequences under saturated repository conditions. Unsaturated conditions may occur in the EDZ in the case of significant gas generation in the EBS. Vapor/air and two-phase flow might be important in the unsaturated zone. However, the major flow and transport pathways are located within the saturated zone. Consequently, these processes have low consequences with the exception of the salt disposal concept. The importance of gas and two-phase flow was demonstrated at WIPP.

This FEP is included as somewhat important to salt in the EDZ and host rock and is excluded from all the other disposal concepts/geologic settings and all the components of the other geologic units based on low consequences.

2.2.12.03 Gas Transport in Geosphere (IS=1, P=0.73)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following processes are included:

- Gas phase transport
- Gas phase release from Geosphere

This FEP is closely related to FEP 2.2.12.01, Gas Generation in Geosphere and FEP2.2.12.02, Effects of Gas on Flow through the Geosphere.

Gas transport in the geosphere can occur either by gas-phase transport in the unsaturated zone or by aqueous-phase transport as dissolved gases in groundwater. Gases that are dissolved in groundwater would be transported by groundwater advection. Dissolved gas may exsolve from aqueous solution into the gaseous phase in the unsaturated zone. Gas may also exsolve if the pressure and temperature change in the geosphere.

The only radionuclides that would have a potential for gas transport are ^{14}C and ^{222}Rn. Rn-222 is a decay product of the ^{238}U-decay series and would be generated for as long as any uranium remained in the repository. Although ^{129}I can exist in the gaseous phase, it is highly soluble, and therefore would be more likely to be dissolved in groundwater rather than exist as a gas. Under saturated repository conditions it is expected that the gas-phase exposure pathways will be of lower importance compared to the aqueous-phase pathways.

This FEP is excluded from all disposal concepts/geologic settings and all the components of the other geologic units based on low consequences.

2.2.14.01 Criticality in Far-Field (IS=1.38, P=0)

This FEP is applicable to all geosphere components, including host rocks, EDZ, and other geologic units. The following process is included:

- Formation of critical configuration

This FEP applies to criticality in the geosphere due to the accumulation of fissile radionuclides (Pu^{239}and/or U^{235}) released from the wastes. Criticality in the geosphere requires the presence of fissionable materials, the presence of a moderator (water), absence of neutron absorbers, the separation of the fissionable material from neutron absorber materials, and the accumulation of a critical mass of fissionable materials separately (since they act as poisons to each other) in a critical geometric configuration.

There is a very low probability that the actinide phases will precipitate in the desired geometry (sphere or cone). Also in many cases the host rocks and the other geologic units contain neutron absorbing materials. This makes assembly of a critical configuration of fissionable material more difficult. Finally, because both, Pu^{239}and U^{235} are present in the wastes and might be present in the groundwater, the poisoning is highly probable.

This FEP is excluded from all disposal concepts/geologic settings and all the components of the other geologic units based on low consequences.

2.3 FEPs Screening Summary

16 out of 51 FEPs were excluded from consideration in the natural system models. These FEPs are summarized in Table 2-1.

35 FEPs were retained because of their importance either to one or more geosphere components (EDZ; Host Rocks; and Other Geologic Units) or one or more disposal concept/geologic settings (Granite; Clay; Salt; and Deep Borehole). The details are provided in Table A-1.

Table 2-1. FEPs Excluded from Natural Systems Models.

NN	FEP NN	FEP Name
1	2.2.05.03	Alteration and Evolution of Geosphere Flow Pathways
2	2.2.07.02	Mechanical Effects on Other Geologic Units
3	2.2.08.07	Mineralogic Dehydration
4	2.2.09.04	Chemical Interactions and Evolution of Groundwater in Other Geologic Units
5	2.2.09.05	Radionuclide Speciation and Solubility in Host Rock
6	2.2.09.06	Radionuclide Speciation and Solubility in Other Geologic Units
7	2.2.09.63	Dilution of Radionuclides with Stable Isotopes
8	2.2.10.01	Microbial Activity in Host Rock
9	2.2.10.02	Microbial Activity in Other Geologic Units
10	2.2.11.03	Thermally-Driven Buoyant Flow / Heat Pipes in Geosphere
11	2.2.11.04	Thermal Effects on Chemistry and Microbial Activity in Geosphere
12	2.2.11.05	Thermal Effects on Transport in Geosphere
13	2.2.11.07	Thermal-Chemical Alteration of Geosphere
14	2.2.12.01	Gas Generation in Geosphere
15	2.2.12.02	Effects of Gas on Flow through the Geosphere
16	2.2.14.01	Criticality in Far-Field

The relationship between the importance to safety case (IS) and overall priority score (P) for the different disposal concepts is shown in Figure 2-2. Note that the IS changes from 1 to 3 and P changes from 0 to 13.

As it can be seen from this figure, only a few FEPs have both, high importance and high or medium priority. Most of the FEPs have low priority, but different levels of importance. Granite has lower importance and priority scores than the other disposal concepts. Salt and clay have greater importance and priority scores than the other disposal concepts. High priority score does not necessarily mean that the FEP is important. It may indicate the lack of information and need for the further research and development.

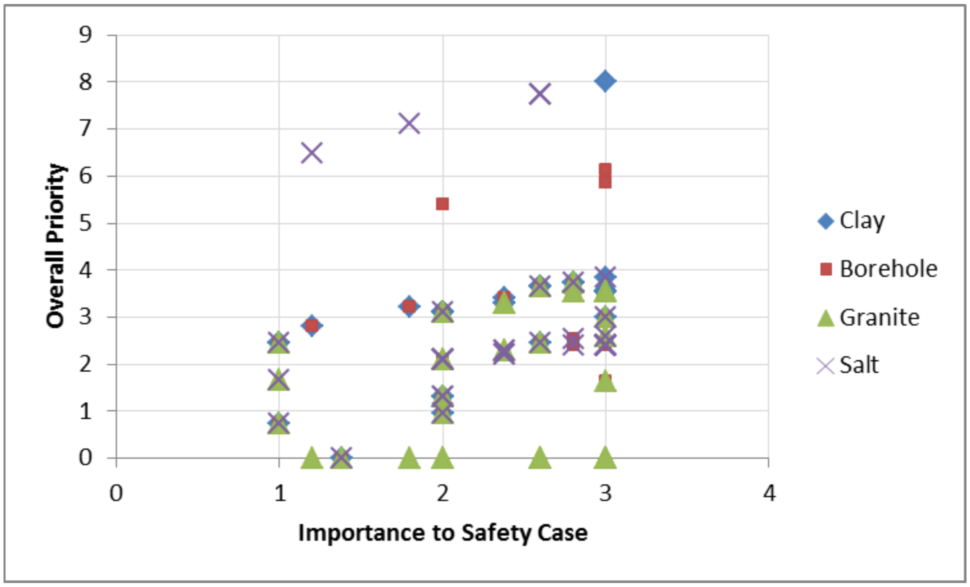


Figure 2-2. Importance to Safety Case and Overall Priority for the Different Disposal Concepts.

2.4 Relationship to EBS and Biosphere FEPs

A number of the Natural Systems FEPs have related FEPs in the adjacent systems, such as Engineered Barrier System (EBS) and Biosphere. The Natural Systems FEPs are also related to the External FEPs that represent conditions other than nominal ones. Table A-1 identifies all the related FEPs.

3. MATHEMATICAL MODELS

3.1 Overview

The generic natural system FEPs identified in Section 2 as important to disposal system performance are used as the basis of the conceptual model used in this element of the GDSM. Mathematical models and the associated governing equations are important components of the conceptual model and are based on the important processes from the FEPs screening. It should be noted that alternative mathematical models exist for some of the processes and several of these alternatives are presented in this chapter (e.g., linear and nonlinear mathematical models of sorption). Generally, simpler alternative mathematical models of important processes can be chosen for the generic natural system model at the current stage of the GDSM.

3.1.1 Continuum Hypothesis

Porous media is comprised of distinct phases and with material properties that change abruptly; however, discrete treatment of porous media geometry is not feasible over length scales of the generic natural system model. Throughout this chapter it is assumed that a representative scale exists over which material properties average out and continuous equations suitably describe the system.

3.1.2 Coupled Systems

Fluid flow in porous media is tightly coupled to the transport of mass and energy in the subsurface. Fluid advection is a very efficient method of transporting dissolved solutes and thermal energy, thus exerts primary control on chemical and temperature distribution in the subsurface. In turn, the fluid chemistry and temperature affect fluid and material properties thus controlling the fluid flow field. The equations given below describe a set of coupled systems affecting the fluid flow, porous media deformation and the transport of dissolved solutes and energy in subsurface.

3.2 Groundwater Flow

If fluid velocities are small and non-turbulent, fluid flow in porous media is described by the compressible, multi-phase form of Darcy's law:

$$\boldsymbol{q_\alpha} = \frac{-\boldsymbol{k}k_{r\alpha}}{\mu_\alpha}(\nabla \boldsymbol{p_\alpha} - \rho_\alpha \boldsymbol{g}) \qquad \textbf{3-1}$$

which gives the fluid flow for phase (α), where $\boldsymbol{k}$ is the permeability tensor and $k_{r\alpha}$ is the relative permeability for a given fluid and phase, p is the fluid phase pressure, μ is the fluid viscosity, and ρ is the fluid phase density.

3.2.1 Permeability Tensor

The permeability of a given porous media is a quantification of the ability for the porous media to transmit fluid. Permeability is a function of the material porosity and the constrictivity of the pore throats. The permeability is directionally dependent and described by a 2nd rank tensor. In stratified sedimentary rocks the bulk permeability of the strata is typically significantly lower in the vertical direction than in the horizontal direction. Permeability changes in space and time, spanning up to eight orders of magnitude. It is the principal controlling parameter for fluid flow and the associated heat and chemical transport in zones of moderate fluid velocity.

3.2.1.1 Relative Permeability and Capillary Pressure

The relative permeability ($k_{r\alpha}$),is an empirical correction which describes the effect of other phases on the effective permeability of a given phase. Both the relative permeability and the capillary pressure are a function of the phase saturation. There are many different empirical models to describe the change of these parameters as a function of saturation. We provide two common examples below.

vanGenuchten-Mualem

The formulation for the relative permeability of the liquid phase is commonly expressed as (van Genuchten 1980):

$$\boldsymbol{k_{rl} = \sqrt{S}\left\{1-\left(1-[S]^{1/m}\right)^{m}\right\}^{2}} \qquad 3\text{-}2$$

and for the gas phase:

$$\boldsymbol{k_{rg} = 1 - k_{rl},} \qquad 3\text{-}3$$

where m is a fitting parameter and S is the effective liquid saturation is given by:

$$\boldsymbol{S = \frac{S_l - S_l^r}{S_l^0 - S_l^r}} \qquad 3\text{-}4$$

where S_l is the residual liquid saturation and S_l^r is the residual saturation and $S_l^0$is the maximum saturation.

The capillary pressure P_c as a function of effective liquid saturation is:

$$\boldsymbol{P_c = {}^{1}/_{\alpha}\left[(S)^{-1/m} - 1\right]^{1/n}} \qquad 3\text{-}5$$

where α, m and n are model parameters and $m = 1 - 1/n$ (van Genuchten 1980.).

Brooks-Corey

Here the liquid relative permeability is given as ():

$$\boldsymbol{k_{rl} = (S)^{(2+3\lambda)/\lambda}} \qquad 3\text{-}6$$

where S is defined by:

$$\boldsymbol{S} = (\boldsymbol{\alpha}|\boldsymbol{P_c}|)^{-\boldsymbol{\lambda}} \qquad 3\text{-}7$$

Thus the capillary pressure is:

$$\boldsymbol{P_c} = \frac{\boldsymbol{1}}{\boldsymbol{\alpha}}(\boldsymbol{S})^{-\boldsymbol{1}/\boldsymbol{\lambda}} \qquad 3\text{-}8$$

andα and λ are the model parameters.

3.2.1.2 Highly Heterogeneous – Fractured Media

The permeability field in geologic systems is variable across spatial scales ranging from the pore scale to formation scales of 100's of km's. As a result of the continuum hypothesis we have assumed a representative scale where permeability is averaged. Several approaches have been used to approximate the effect of heterogeneity in the averaged parameter which generally tends to include a stagnant or low permeability volume associated with each representative elementary volume. The exchange of fluid and solutes between the active and immobile zone is described to varying degrees.

Dual Porosity

In the double-porosity model the subsurface is divided into a mobile and immobile domain. Advection and dispersion occur in the mobile zone only, and solute is exchanged with the immobile porosity via a first order exchange based on the solute concentration gradient (Sudicky 1990, Sudicky& McLaren 1992).

Dual Continuum

A highly mobile (fracture) continuum interacts with a porous media matrix continuum with regard to fluid flow and solute transport. Flow, dispersion and diffusion occur in both media. No gradients are captured within the matrix nodes (Sudicky 1990, Sudicky& McLaren 1992).

Multiple Interacting Continuum

Fractures are lumped into continuum #1 and then multiple matrix continua are applied to increasing matrix distance from the fracture continuum (Pruess 1985). The use of multiple continua allows for the capture of gradient from the fractures into the matrix. Advection, dispersion and diffusion occur in all continua.

3.2.2 Time Variance

Groundwater flow can change as a function of time at a variety of temporal and spatial scales in response to changing boundary conditions. Examples include variations in recharge with changing climate and changing patterns of groundwater pumping. In addition, long-term changes in parameters within the governing equations, such as permeability, can occur in response to coupled chemical and mechanical processes.

Reaction

Chemical reactions involving mineral phases include dissolution and precipitation which change formation porosity and therefore can change permeability as a function of time. Such changes can be the result of natural hydrogeolgical evolution of the system or, more locally, as a result of the thermal and chemical perturbations from the presence of the repository.

Tectonics

Tectonic forces can cause changes in the permeability field over geologic time scales due to changes in pressure as a result of burial and/or exhumation and changes in the stress field cause compaction or expansion. Over shorter time scales seismic rupture and faulting can cause rapid changes in the permeability field. Seismic effects may be naturally reversible over time scales that are short relative to repository performance.

3.2.3 General Multiphase Flow

Conservation of mass combined with equation 3-1 gives the generalized multicomponent, multiphase flow equation:

$$\frac{\partial}{\partial t}\left(\phi \sum_\alpha \rho_\alpha s_\alpha Y_{j\alpha}\right) + \nabla \cdot \left(\sum_\alpha \frac{-\boldsymbol{k} k_{\boldsymbol{r\alpha}} \rho_\alpha Y_{j\alpha}}{\boldsymbol{\mu_\alpha}} \boldsymbol{\nabla}(p_\alpha - \rho_\alpha \boldsymbol{g})\right) = Q_j \qquad \text{3-9}$$

where s_α is the phase saturation, $Y_{j\alpha}$ the mass fraction for component j in the phase, $\boldsymbol{k}$ is the intrinsic permeability, $k_{\boldsymbol{r\alpha}}$ is the relative permeability of the phase, s_α and ρ_α are the saturation and density of the phase respectively, $\mu_{\boldsymbol{\alpha}}$ is the viscosity of the phase, and Q_j is the source term for the component j (Steefel 2010, Wang et al. 2011). Gas phase sources that may be relevant to nuclear waste disposal include corrosion, radiolysis, and biodegradation; however, these sources are probably less relevant to the natural system than to flow in the EBS. If significant gas phase sources are present, numerical solution of the non-linear governing equations may be additionally challenging.

3.3 Heat Transport

3.3.1 Conservation of Energy

The flow of fluid is given by equation 3-9. The coupled multiphase heat transport equation is governed by:

$$\boldsymbol{\frac{\partial\left[\phi \rho_\alpha s_\alpha Y_{j\alpha} H_\alpha + (1-\phi)\rho_\alpha H_r\right]}{\partial t} + \nabla \cdot \sum_\alpha \frac{-k k_{r\alpha} \rho_\alpha Y_{j\alpha} H_\alpha}{\mu_\alpha} \nabla(p_\alpha - \rho_\alpha g) - \nabla \cdot K_m \nabla T = Q_h} \qquad \text{3-10}$$

where H_α is the fluid phase enthalpy, H_r is the enthalpy of the rock mass, K_m is the thermal conductivity and T is the porous media temperature with the assumption that fluid and rock temperatures are in equilibrium and Q_h are heat sources and sinks (Ingebritsen et al. 2006). The first term in equation 3-10 considers the change in energy storage with time, the second term is the advective heat transport while the third term considers heat transport via conduction. Equations 3-9 and 3-10 are a set of coupled equations where heat transport can occurs by fluid advection, and thermal energy affects the fluid flow via fluid potential and properties are considered.

3.4 Solute Transport

3.4.1 Conservation of Mass

The general form for multiphase transport in porous media is given by:

$$\boldsymbol{w_m}\left[\frac{\boldsymbol{\partial[\phi\sum_\alpha C_\alpha s_\alpha]}}{\boldsymbol{\partial t}}\right]-\boldsymbol{\nabla\cdot w_m}\sum_{\boldsymbol{\alpha}}\boldsymbol{q_\alpha C_\alpha s_\alpha}-\boldsymbol{\nabla}$$

$$\boldsymbol{\cdot\, w_m\sum_\alpha s_\alpha\, D_\alpha^e\phi\nabla C_\alpha}+\boldsymbol{\sum_\Omega J_{ex}}=\boldsymbol{Q_i} \qquad \text{3-11}$$

where w_m is the volumetric fraction of total porosity that is mobile, C_α is the concentration of the solute in phase α, q_α is the darcy velocity of phase α which is given by equation 3-9, D_α^e is the effective dispersion coefficient, J_{ex} is the exchange flux between the different domains supported by the model and Q_i represents sources and sinks of solutes including reaction, sorption and external sources (Steefel 2010, Wang et al. 2011). The first term in equation 3-11 described the mass change with time of solute i, the second term describes the advective transport, the third term the dispersive transport, the fourth term the exchange between multiple domains within the model and the fifth is a general term for the many forms of subsurface sources and sinks. Equations 3-9 and 3-11 are coupled by inclusion of q_α in equation 3-11, while the concentration of solute can change the fluid density and the porous media properties, thus affecting the flow.

3.4.2 Advection

Fluid movement is directly controlled by the permeability tensor and relative permeability curves for the given phase. In systems with moderate fluid velocities, advective transport is the dominant form of solute transport, thus parameterization of the permeability field is a primary concern for prediction of solute transport.

3.4.3 Dispersion

Mechanical dispersion accounts for small variations in fluid velocity at the pore scale, the tortuous path solutes take through porous media, and small scale heterogeneity. Thus the linear transport velocity of a solute varies around a mean velocity. If the velocity variance is normally distributed dispersion can be modeled as a Fickian process, giving the classic form of the advection dispersion equation in 3-11. If Fickian behavior is assumed, both mechanical dispersion and diffusion operate in the same fashion and their effect can be combined into hydrodynamic dispersion where the hydrodynamic dispersion tensor is given by:

$$\boldsymbol{D^{e}_{\alpha_{ij}} = \xi_{ijkl}\frac{v_k v_l}{|v|} + D'_{m_\alpha}}, \qquad \boldsymbol{i, j, k, l = 1 \ldots .\, n_d} \tag{3-12}$$

where $D^{e}_{\alpha_{ij}}$ is the effective hydrodynamic dispersion coefficient, ξ_{ijkl} is the fourth order dispersivity tensor, v_k and v_l are the spatial components of the velocity, $|v|$ is the magnitude of the velocity vector. For an isotopic medium the fourth order tensor of dispersivity reduces to two components, a longitudinal:

$$\boldsymbol{D_L = \xi_L v_L + D'_{m_\alpha}} \tag{3-13}$$

and transverse:

$$\boldsymbol{D_T = \xi_T v_L + D'_{m_\alpha}} \tag{3-14}$$

where L is the main axis of solute migration and v_L is the mean fluid velocity along that direction. Mechanical dispersion reflects our ignorance of the velocity field. As the scale of investigation increases, our ignorance of the permeability distribution and velocity field increases, thus measured dispersivity coefficients increase with the scale of measurement.

3.4.4 Diffusion in Porous Media

The effective diffusion coefficient for a solute in porous media is affected by the effective porosity, the tortuosity, multiphase effects and charge balance for multiple species giving:

$$\boldsymbol{D'_m = \phi_e \tau D_m} \tag{3-15}$$

where ϕ_e is the effective porosity, τ is the tortuosity and D_m is the free solution diffusion coefficient. The effective porosity is the pore volume available to a given ionic species, and is affected by mineral surface charge, ion charge and the ionic strength of the solution. The tortuosity accounts for the diffusion path around mineral grains being longer than the linear distance traveled. In high ionic strength, multi-component systems, charge balance must be maintained and electrochemical migration must be considered.

3.4.5 Matrix Diffusion

In geologic media with highly heterogeneous permeability groundwater flow will occur dominantly in zones of high permeability and flow will be minimal in zones of low permeability.

This process is particularly important to flow and solute transport in fractured porous media, but may also apply to a system of aquifers and confining units.

3.4.5.1 Mobile – Immobile Zone

If the contrast in permeability between the fracture network and the rock matrix is sufficiently large (e.g., greater than three or four orders of magnitude), then the fractured porous media can be approximated as consisting of two zones, a mobile zone and an immobile zone. Groundwater flow is assumed to occur only in the mobile zone and diffusive mass transfer of solutes can occur between the mobile zone (fractures) and the immobile zone (matrix). Although realistic fracture networks are geometrically complex, the simplifying assumption of one-dimensional diffusion in the matrix is often used in mathematical models of matrix diffusion (e.g., Sudicky and Frind, 1982).

3.4.5.2 Dual Porosity

Diffusion between the mobile and immobile zones, and diffusion within the immobile zone is governed by Fick's Law, as expressed in the following equations:

$$\boldsymbol{J_{ex} = -D_m' \frac{dC}{dz}} \qquad \text{3-16}$$

where J_{ex} is the general exchange flux of solute between the mobile and immobile zones from equation 3-11 and z is the direction into the immobile zone perpendicular to the zone boundary. Diffusion within the immobile zone (matrix) is governed by:

$$\boldsymbol{\frac{\partial C}{\partial t} = \frac{D_m'}{K_d \rho_s} \frac{\partial^2 C}{\partial z^2}} \qquad \text{3-17}$$

where t is time, K_d is the linear sorption coefficient, and ρ_s is the bulk density of the matrix.

3.4.5.3 Multi-Rate Diffusion

Heterogeneity in matrix block size, fracture surface area, and matrix pore-scale geometry exists in fractured porous media, leading to complexity in the process of matrix diffusion. Generalized conceptual and mathematical models of the multiple rates of solute mass transfer between the mobile and immobile zones that accounts for such heterogeneity have been developed by Haggerty and Gorelick (1995). The multi-rate diffusion model has been shown to more closely match tracer breakthrough curves for tracer tests conducted in fractured dolomite (McKenna et al., 2001). In this conceptualization the single value of diffusion rate coefficient used in the dual porosity model is replaced with a lognormal probability density function of the diffusion coefficient, $\boldsymbol{b(\alpha_d)}$, as shown in Haggerty and Gorelick (1998):

$$\boldsymbol{b(\alpha_d) = \frac{\beta_{\text{tot}}}{\sqrt{2\pi}\sigma_d\alpha_d} \exp\left\{\frac{[\ln(\alpha_d) - \mu_d]^2}{2{\sigma_d}^2}\right\}}, \qquad \text{3-18}$$

where:

$$\alpha_d = \frac{D_m'}{l^2}, \tag{3-19}$$

$$\beta_{\text{tot}} = \frac{\varphi_d R_d}{\varphi_a R_a}, \tag{3-20}$$

where β_{tot} is the total capacity coefficient, σ_d is the standard deviation of the log-transformed diffusion rate, α_d is the continuously distributed diffusion rate coefficient, μ_d is the mean of the log-transformed diffusion rate coefficient, l is the length of the diffusion pathway in the matrix, φ_d is the matrix porosity, φ_a is the advective porosity, R_d is the retardation factor in the matrix, and R_a is the retardation factor in the advective porosity.

3.4.6 Biogeochemical Reactions

Biogeochemical reactions are contained in the source terms of equation 3-11. Thus reactive transport must consider chemical reaction along the flow path. A chemical system of N species and N_r reactions can be separated into N_c primary species A_j and N_x secondary species A_i. The equilibrium chemical reactions can be written (Kirkner, D.J):

$$A_i \Leftrightarrow \sum_{j=1}^{N_c} v_{ij} Aj \;\;,\;\; j = 1, \dots, N_c \tag{3-21}$$

where v_{ij} is number of moles of primary species j in secondary species i. The equilibrium concentrations are given by N_x mass action equations:

$$C_i = \frac{\prod_j^{N_c} (C_j \gamma_j)^{v_{ij}}}{\gamma_i K_i} \tag{3-22}$$

where C_i, γ_i and C_j, γ_j are the concentration and activity coefficients of the secondary and primary species respectively.

3.4.6.1 *Kinetic Reactions*

The general mass balance equation for kinetic transport can be written:

$$\frac{\partial}{\partial t}(\phi s_\alpha C_i) + \nabla \cdot J_i = \sum_{r=1}^{N_r} v_{ir} I_r \quad (i = 1, \dots . N) \tag{3-23}$$

where J_i is the transport flux, v_{ir} is the number of moles i participating in and I_r is the reaction rate for reaction r. Solving equation 3-22 is difficult due to incomplete knowledge of reaction rates, large variations in reaction rates between homogenous and heterogeneous reactions and large differences in concentrations, so simplifying assumptions must be made. Common assumptions include local equilibrium which is equivalent to transported batch reactions and is suitable only in situations where transport time is much longer than even the slowest reaction time scale (Reeves & Kirkner 1988). Local partial equilibrium essentially divides the system into slow and fast reaction, and considers fast reactions to be equilibrium reactions and thus only need consider slow reactions kinetically (Lichtner,).

3.4.6.2 *Activity Coefficients*

The activity coefficients in equation 3-12 describe the difference of the chemical activities of a solute in the thermodynamic sense and the actual concentration and can be calculated using a variety of methods which fall into two distinct methods (Wang et al. 2011). The first method takes into account long-range ionic interactions and includes Debye-Huckel, Davies and B-dot models, which are applicable over differing ranges of ionic strength (Bethke,). The second method is the “Pitzer” method (Pitzer 1979) which considers little or no speciation, because short range interactions dominate at high ionic strengths, thus the Pitzer method is applicable only in high ionic strength solutions (Wang et al. 2011).

3.4.7 Sorption

Sorption is the attachment or complexation of solutes with mineral surfaces. The sorption process can be described with various degrees of fidelity from simple empirical formulations to more complex mechanistic ones (Drever,).

3.4.7.1 *Linear Isotherm*

The simplest way to describe sorption is to treat it like an equilibrium reaction which is described by:

$$\boldsymbol{C_{i(ads)} = K_d C_{i(aq)}} \qquad 3\text{-}24$$

where the adsorbed concentration ($C_{i(ads)}$mol/kg$_s$) is linearly related to the aqueous concentration ($C_{i(aq)}$ mol/L). This method is attractive because of its simplicity and low computational cost in solute transport codes.

3.4.7.2 *Freunlich Isotherm*

Here sorption is modeled as an exponential relationship:

$$\boldsymbol{C_{i(ads)} = K_f C^{n}_{i(aq)}} \qquad 3\text{-}25$$

where n is a constant that is usually less than 1. The Freundlich isotherm can be regarded as strictly empirical relation which could result from heterogeneity in material properties (Drever,).

3.4.7.3 Langmuir Isotherm

In the Langmuir model of the sorption reaction is written as:

$$\boldsymbol{C_{i(ads)} = K_f C_{i(aq)} C_{vac}} \qquad 3\text{-}26$$

where C_{vac} is the concentration (mol/L) of vacant sorption sites on the mineral surface. Sorption models of increasing complexity can be modeled including multi-site, multi-component exchange (Appelo&Postma 1993), which require more data and increasing computational power.

3.4.8 Mineral Precipitation and Dissolution

A geochemical reaction is described as an overall reaction with unknown intermediate steps. Thus, the measured empirical rate constant for a mineral-water reaction can be formulated (Lichtner,):

$$\boldsymbol{I_m = s_m k_m \prod_i a_i^{\beta_i} f(\Omega_m)} \qquad 3\text{-}27$$

where k_m is the reaction rate constant; s_m is the surface area of mineral m; a_i is the activity of species i; and Ω_m is the saturation degree of the solution with respect to mineral m. In general, the reaction rate is a nonlinear function of the concentrations of dissolved species.

Microbially mediated reactions have been described as:

$$\boldsymbol{I_m = I_{max}\left(\frac{C_D}{K_D + C_D}\right)\left(\frac{C_A}{K_A + C_A}\right)} \qquad 3\text{-}28$$

where C_D and C_A are the concentrations of electron donor and acceptor respectively; and K_D and K_A are the half-saturation constants for electron donor and acceptor respectively(Wang & Papenguth 2001).

3.4.9 Colloidal Transport

Colloids are small organic and inorganic particles from 1nm – 1μm in size. Colloids can provide mobile surface areas. Solutes adsorped to these colloids can be carried along with transported colloids. Colloid facilitated transport is thus affected by the partitioning of solutes to colloids and parameters controlling colloid transport such as retardation rates for colloids and filtration. The filtration coefficient ε is given by (Harvey, R.W.):

$$\boldsymbol{\varepsilon = 1.5\frac{1-\phi}{d_m}\alpha_c\eta_c}\,, \tag{3-29}$$

where

$$\boldsymbol{\eta_c = 0.9\left(\frac{k_BT}{\mu d_c d_m q}\right) + 1.5\left(\frac{d_c}{d_m}\right)^2 + (\rho_c - \rho)\frac{gd_c^2}{12\mu q}} \tag{3-30}$$

where d_m is the particle size of the medium grains; α_c is the collision efficiency factor; η_c is the single collector efficiency; d_c is the colloid diameter, k_B is the Boltzmann constant; T is the absolute temperature; ρ_c is the colloid density; ρ is the water density; μ is the water viscosity; q is the Darcy velocity; and g is the gravity constant.

3.5 Geomechanics

For a static geomechanical process force equilibrium gives:

$$\boldsymbol{\nabla\cdot\sigma = 0} \tag{3-31}$$

where $\boldsymbol{\sigma}$ is the 2nd order total force tensor. For porous media the effective stress tensor is defined by (Ingebritsen et al. 2006):

$$\boldsymbol{\sigma' = \sigma - \alpha P} \tag{3-32}$$

where P is the porefluid pressure and $\alpha = 1 - c_s/c_b$ where c is the compressibility of the mineral grains (s) and porous media (b). The strain tensor ($\boldsymbol{\varepsilon}$) can be defined by (Steefel 2010):

$$\boldsymbol{\varepsilon = \frac{1}{2}((\nabla u)^T + \nabla u)} \tag{3-33}$$

where $\boldsymbol{u}$ is the displacement vector. Equations 3-32 and 3-33 are related through the constitutive response of the deformation material. These responses range from simple elastic to more complex relationships such as elasto-plastic deformation. Using the constitutive relationship for elastic media the equation describing deformation in a thermoelastic porous media is (Ingebritsen et al. 2006):

$$\boldsymbol{G\nabla^2 u + \frac{G}{1-2v}\nabla(\nabla\cdot u) = \alpha\nabla\frac{\partial P}{\partial t} + G\frac{2(1+v)}{1-2v}\alpha_T\nabla\frac{\partial T}{\partial t}} \tag{3-34}$$

where G is the shear modulus, v is Poisson’s ratio and α_T is the thermal expansion coefficient of the porous media.

For simplicity we consider a single phase flow system and couple equation 3-34 to porous media flow via displacement in the storage term:

$$\boldsymbol{\nabla\cdot\left[\frac{k\rho_f g}{\mu_f}\nabla\left(P+\rho_f g\right)\right] = s'_{S3}\frac{\partial P}{\partial t} - \rho_f g\alpha\frac{\partial}{\partial t}(\nabla\cdot u) - \rho_f g\Lambda\frac{\partial T}{\partial t}} \tag{3-35}$$

where $s'_{S3}$is the specific storage and Λ is the thermal response coefficient given by $\Lambda = \alpha_{Tf} - \alpha_T$ where α_{Tf} is the linear coefficient of thermal expansion for the fluid. The specific storage is given by:

$$\boldsymbol{s'_{S3} = \rho_f g\left[(\alpha+1)(c_b - c_s) + \left(nc_f - nc_s\right)\right]} \tag{3-36}$$

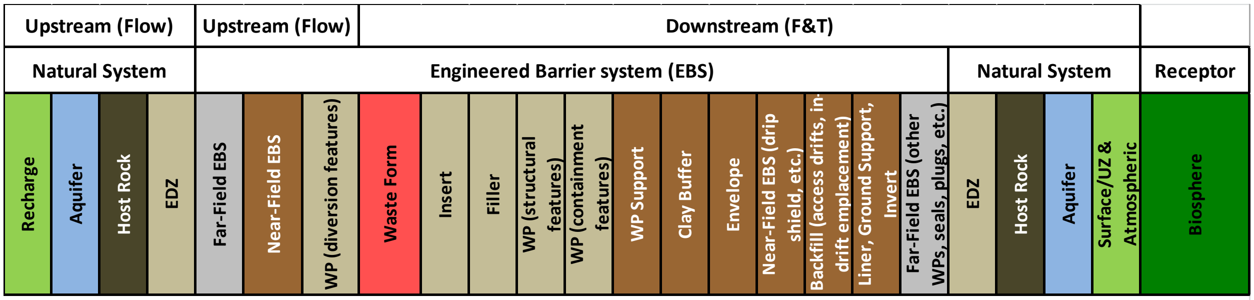
where c_f is the fluid compressibility. The fluid flow equations provide changes in pressure with time which affect the porous media displacement via the pressure terms in equation 3-34, and the deformation of the porous media effects fluid flow via the displacement term on the right hand side of equation 3-35.

4. GENERIC CONCEPTUAL MODEL

4.1 Generic Hydrogeologic Setting for Disposal System Alternatives

The generic natural system conceptual model consists of a three-dimensional domain that has sufficient spatial extent to contain all significant hydrological, thermal, and mechanical perturbations caused by the presence of the repository. The conceptual model domain must also contain the assumed interface with the biosphere. Ideally, the model domain would extend to natural groundwater flow boundary conditions, such as no-flow groundwater divides and surface discharge locations, zero-flux confining units at the lower boundary, and natural recharge conditions at the topographic surface.

The generic natural system model is conceptually divided into subdomains consisting of the engineered disturbed zone (EDZ) (or disturbed rock zone), the host rock, the aquifer system, and the surface/unsaturated zone (UZ) and atmospheric system, as shown in Figure 4-1 (Hardin 2012). These subdomains may be subdivided or combined in terms of hydrogeologic units depending on the disposal system alternative or site-specific geology. For example, the host rock, aquifer system, and UZ system may all be a single fractured granite bedrock hydrogeologic unit in the case of a mined repository in crystalline rock. For a clay or salt repository, the aquifer system may consist of several distinct hydrogeologic units that correspond to multiple aquifers and aquitards in the stratified sedimentary system overlying the repository.



Upstream (Flow)				Upstream (Flow)			Downstream (F&T)																
Natural System				Engineered Barrier system (EBS)															Natural System				Receptor
Recharge	Aquifer	Host Rock	EDZ	Far-Field EBS	Near-Field EBS	WP (diversion features)	Waste Form	Insert	Filler	WP (structural features)	WP (containment features)	WP Support	Clay Buffer	Envelope	Near-Field EBS (drip shield, etc.)	Backfill (access drifts, in-drift emplacement)	Liner, Ground Support, Invert	Far-Field EBS (other WPs, seals, plugs, etc.)	EDZ	Host Rock	Aquifer	Surface/UZ & Atmospheric	Biosphere

Notes:

1. Clay Buffer = Includes reservoir used to manage heat and/or multiphase flow around waste packages
2. Envelope = container for pre-fab. EBS

Figure 4-1. System Model Architecture (from Hardin, 2012).

A summary of the generic natural system conceptual model for the four alternative disposal systems is shown in Table 4-1.

Table 4-1. Summary of the Generic Natural System Conceptual Model.

Conceptual Model Component	**Crystalline Rock Repository**	**Salt Repository**	**Clay Repository**	**Deep Borehole Disposal**
Approximate Domain Dimensions	30 km by 20 km by 1 km depth	30 km by 20 km by 1 km depth	30 km by 20 km by 1 km depth	10 km by 10 km by 6 km depth
Hydrogeologic Framework	Fractured granite and granitic gneiss bedrock, sparse vertical shear zones of enhanced permeability, overlying variable thin (<100 m thick) alluvial aquifer	Basal 400-m thick siltstone-shale unit, 200-m thick bedded salt host rock, overlying 300-m thick siltstone-shale unit, uppermost 100-m thick fractured carbonate aquifer, all units horizontal	Basal 200-m thick shale unit, 200-m thick sandstone aquifer unit, 200-m thick clay-shale host rock, 200-m thick overlying siltstone unit, uppermost 200-m thick sandstone aquifer, all units horizontal	5000-m thick fractured granite and granitic gneiss host rock and crystalline basement, sparse vertical shear zones of enhanced permeability, upper 1000 m sedimentary rocks consist of alternating 100-m thick sandstones, shales, and fractured carbonate units, all sedimentary units horizontal
Initial Conditions	Steady-state hydrologic, thermal and mechanical conditions for ambient configuration	Steady-state hydrologic, thermal and mechanical conditions for ambient configuration	Steady-state hydrologic, thermal and mechanical conditions for ambient configuration	Steady-state hydrologic, thermal and mechanical conditions for ambient configuration
Groundwater Boundary Conditions	No-flow specified for lower and lateral boundaries, specified recharge flux at top boundary, specified head corresponding to location of natural discharge area at lower-elevation end of top boundary, average	No-flow specified for lower and lateral boundaries, specified recharge flux at top boundary, specified head corresponding to location of natural discharge area at lower-elevation end of top boundary, average	No-flow specified for lower and lateral boundaries, specified recharge flux at top boundary, specified head corresponding to location of natural discharge area at lower-elevation end of top boundary, average	No-flow lower boundary, specified hydrostatic pressure on lateral boundaries, specified atmospheric pressure at top boundary, zero horizontal and vertical gradients

	horizontal gradient of 0.001.	horizontal gradient of 0.001.	horizontal gradient of 0.001.	
Thermal Boundary Conditions	Specified heat flux for lower boundary, specified temperature for side and top boundaries	Specified heat flux for lower boundary, specified temperature for side and top boundaries	Specified heat flux for lower boundary, specified temperature for side and top boundaries	Specified heat flux for lower boundary, specified temperature for side and top boundaries
Mechanical Boundary Conditions	Specified zero vertical displacement on lower boundary, specified horizontal stress on side boundaries, specified zero vertical stress on top boundary	Specified zero vertical displacement on lower boundary, specified horizontal stress on side boundaries, specified zero vertical stress on top boundary	Specified zero vertical displacement on lower boundary, specified horizontal stress on side boundaries, specified zero vertical stress on top boundary	Specified zero vertical displacement on lower boundary, specified horizontal stress on side boundaries, specified zero vertical stress on top boundary
Flow and Transport Processes	Heterogeneous continuum for groundwater flow and dual-porosity approach for transport in fractured media	Heterogeneous continuum for groundwater flow and dual-porosity approach for transport in fractured media	Heterogeneous continuum for groundwater flow and dual-porosity approach for transport in fractured media	Heterogeneous continuum for groundwater flow and dual-porosity approach for transport in fractured media
Governing Equations	See Section 3	See Section 3	See Section 3	See Section 3

4.1.1 Hydrogeologic Framework

Specifics of the hydrogeologic framework for natural system modeling, including stratigraphy, lithology, and structural geology, are highly variable and site specific. Nonetheless, meaningful generalizations can be made about the hydrogeologic framework for the four disposal system options, for the purposes of the generic natural system conceptual model. These generalizations are made on the basis of geological associations between the genesis of the host rock and other geological units.

Bedded salt forms by the evaporation of seawater on the shallow margins of sedimentary basins, in which the circulation of seawater was restricted enough to allow the precipitation of evaporite minerals. Such low-energy depositional environments also result in the sedimentary deposition of fine grained clastic sediments such as clay and silt, so bedded salt deposits are generally interspersed with shales and siltstones. Continuing evolution of the sedimentary basin eventually leads to greater circulation of seawater along the basin margins, and evaporite deposits are often overlain by carbonate rocks, sandstone, and additional fine-grained strata. The generic hydrogeologic framework for the salt repository thus consists of underlying shales and siltstones, salt host rock, overlying shales, and an upper fractured carbonate rock aquifer. This conceptual model approximately corresponds to the geology of the WIPP site in the Permian Basin of New Mexico.

The crystalline rock repository concept encompasses a range of potential rock types; however, most sites that have been investigated for a crystalline rock repository have consisted of felsic igneous and metamorphic rocks, such as granite and granitic gneiss. Such Precambrian rocks are widespread, typically moderately to sparsely fractured, and include widely spaced fracture or shear zones of enhanced permeability. The hydrogeologic framework for the crystalline rock repository option consists of fractured granite or granite gneiss, with a relatively thin (<100 m thick) alluvial aquifer overlying the granite. This conceptual hydrogeologic framework approximately corresponds to the geology of the SKB-3 concept (SKB 2006).

Clay, shale, or argillite rocks that are appropriate for the clay repository disposal system can form in a variety of sedimentary environments, ranging from a deep marine setting to lake beds. While the depositional environment for these fine-grained sediments is very low energy, underlying and overlying strata may be coarser grained clastic sediments from near shore and terrestrial depositional environments, and it is difficult to draw generalized conclusions about their lithology. The hydrogeologic framework for the clay repository consists of an underlying sandstone unit, a thick clay-shale host rock, overlying siltstone, and uppermost sandstone unit.

The assumed hydrogeologic framework for the deep borehole disposal concept extends to a much greater depth than the mined repository concepts and consists of deeper crystalline basement rocks and sedimentary rocks in the upper 1000 m of the model. The crystalline rock consists of fractured granite or granite gneiss with widely spaced fracture zones of enhanced permeability. The sedimentary section consists of alternating sandstones, shales, and carbonate units.

4.1.2 Initial Conditions

Steady-state, equilibrium conditions for groundwater flow, heat flow, and mechanical stress are justifiable as the initial conditions for the generic natural system model for the four alternative disposal systems, with some possible exceptions for some sites. Ambient conditions in the natural system may be altered somewhat by dewatering within or stress redistribution around the repository excavation, but such perturbations generally occur only very near the EBS. Non-equilibrium conditions may have persisted to the present day following continental glaciation in very low permeability units, such as overpressured conditions in clay or shale. Post-glacial rebound would also lead to non-steady state hydrologic and mechanical conditions for slowly rising landscapes. Variations in past climatic conditions can also result in non-equilibrium temperature profiles with depth. None of these transient effects would have significant impacts on the generic natural system model with regard to simulations of radionuclide transport from repository systems.

4.1.3 Boundary Conditions

Defining the boundary conditions for any model of the natural system is an important component of developing the conceptual model because the overall behavior of the model is largely determined by those boundary conditions. Typically, site-specific information and inferences about groundwater flow systems in general, for example, are used in defining the boundary conditions. Boundary conditions for the generic natural system model are arbitrary in the sense that the model does not correspond to any specific site. Nonetheless, reasonable assumptions about the boundary conditions can be made on the basis of “typical” natural system characteristics and assuming that a site with generally favorable characteristics would be chosen for a repository disposal system.

Groundwater boundary conditions for the three mined repository concepts are defined for the generic natural system model assuming a sub-regional flow system with dimensions of 20 km by 30 km, with significant active groundwater flow extending to a depth of 1 km (see Table 4-1). Groundwater flow is driven by distributed recharge on the topographic surface and surface water discharge at one end of the flow system, resulting in relatively low average horizontal hydraulic gradient of 0.001. Such a groundwater flow system corresponds to an area with limited topographic relief, low-permeability rocks below 1 km, and lack of large-scale, regional groundwater driving forces.

Groundwater boundary conditions for the borehole disposal system are defined for a flow system with no vertical fluid driving forces (i.e., without overpressured or underpressured conditions at depth). Lateral boundaries consist of specified hydrostatic pressure, allowing inflow and outflow of groundwater in response to thermally induced convection resulting from waste heat. No significant horizontal hydraulic gradient is assigned to the shallow part of the model domain. These boundary conditions correspond to a stable continental interior location with stagnant groundwater in the deep crystalline basement and no significant flow in the overlying sedimentary rock cover.

Thermal and mechanical boundary conditions assigned to the generic natural system model are the same for all four disposal system alternatives. The thermal and mechanical boundary conditions are far enough from the repository or disposal boreholes that they have little impact on the temperature and stress calculations related to waste heat. These boundary conditions correspond to a location with low to moderate heat flow in a tectonically stable environment without a large differential in ambient horizontal stress.

4.2 Generic Release Scenarios

Generic release scenarios for the natural system model include nominal and disruptive cases. The nominal case is summarized in the conceptual model description in this section of the report and the anticipated disruptive cases can be accommodated with achievable modifications of the nominal case generic natural system model. The human intrusion disruptive case typically entails hypothetical future drilling into the repository and creating a mechanism for radionuclide release that bypasses some or all of the barriers in the EBS and natural system. The generic natural system model could be modified to include direct release of radionuclide mass into the natural system at any location along the drill hole for the human intrusion release scenario. The seismic disruptive case could include activation of faults in the natural system and enhanced permeability in fracture networks and along faults following an earthquake. The seismic release scenario could be accommodated in the generic natural system model by changing values of permeability and the nature of heterogeneities in the natural system. If continental glaciation is a plausible disruptive event at a particular site, impacts on the natural system would include increased fluid pressures, alteration of groundwater boundary conditions, increased vertical mechanical stress, and suppressed temperatures in the geothermal gradient. Modifications of the nominal generic natural system model could include these changes, although complex thermal-hydrological-mechanical coupling would probably require more advanced numerical simulation methods.

4.3 Interfaces with the EBS and the Biosphere

The interfaces between the generic natural system model and the EBS and biosphere must be defined conceptually, geometrically, and with regard to the exchange of information on radionuclide transport. The nature of these interfaces has important implications for consistency among the components of the GDSM and for the overall capabilities of the GDSM.

The geometry of the interface between the generic EBS model and the generic natural system model can be abstracted as a simplified representation or as a geometrically realistic representation of the repository design. For mined repository systems a simplified representation would be a rectangular prism embedded within the generic natural system model that has homogeneous, average hydrologic, thermal, and mechanical properties representative of the entire EBS. Similarly, the EBS in this simplified representation would be treated as a uniform source term for radionuclides released from the repository. For the deep borehole disposal system it is probably necessary to represent individual boreholes in an array of boreholes for the interface between the generic EBS model and the generic natural system model. The EDZ would be included as a “skin” surrounding the simplified rectangular prism representing the EBS. A geometrically more realistic interface between the generic EBS model and the generic natural system model would include individual waste disposal drifts of the repository. The radionuclide source term would include releases from specific locations at the interface, based on detailed simulation results from the generic EBS model. The complexity of the interface between the generic EBS model and the generic natural system model would be commensurate with the complexity and spatial resolution of both component models. Explicit representation of individual repository drifts would require high-resolution gridding in both the generic EBS model and the generic natural system model, and would probably require high-performance computing for the numerical implementation of such a conceptual model. Routine probabilistic calculations with the GDSM do not require this level of fidelity.

The interface between the generic EBS model and the generic natural system model must also be defined in terms of groundwater flow, radionuclide transport, heat flux, and mechanical stress or displacement. Groundwater flow between the EBS and the natural system should be fairly limited as long as the buffer materials, grouting, and repository seals remain effective in the mined repository systems. For the deep borehole disposal system there would be more interaction between fluids in the host rock and the EBS in the disposal zone. In either case, the interface between the generic EBS model and the generic natural system model should allow for groundwater flow between the two GDSM components. Radionuclide transport between the EBS and the natural system would be controlled by both advective transport and diffusive transport, with diffusive transport dominating for the nominal scenario in the mined repository systems. Unidirectional transport from the EBS to the natural system is a justifiable simplification and would be implemented with a specified radionuclide flux coupling between the two component models. Thermal coupling between the generic EBS model and the generic natural system model should be bidirectional to obtain accurate estimates of near-field temperature history in the EBS. In the case of the deep borehole disposal system bidirectional coupling of heat transport at the interface between the EBS and natural system is particularly important because of the role in thermal-hydrologic effects in driving groundwater flow. Mechanical and thermo-mechanical effects are probably less important for the generic natural system model and could be implemented in a simplified, unidirectional fashion.

Numerous potential scenarios are plausible for the release of radionuclides to the biosphere. Releases could occur at natural groundwater discharge locations, such as springs, rivers, lakes, or the ocean. More directly, radionuclide releases could occur in a hypothetical future pumping well that supplies groundwater for drinking, household use, and/or agriculture. For simplicity and given current regulations, the pumping well release scenario should be used for the generic natural system model in the GDSM. This form of the interface between the natural system and the biosphere also avoids the technical uncertainties and numerical limitations associated with accurately simulating *in situ* radionuclide concentrations in groundwater or in surface water bodies that have received contaminated discharge.

4.4 Transience in the Natural System

The natural system may experience transient conditions for different features and processes over a range of time scales. Groundwater flow conditions change at short time scales in response to individual precipitation events, seasonal variations in precipitation and evapotranspiration, and variations in river stage, lake levels, or marine tidal conditions. In addition, the presence of a mined repository and dewatering of the excavation may impact local groundwater flow rates and directions in the natural system. Such short term transience in groundwater flow is generally limited to the shallowest parts of the flow system or near the repository for a short period of time, has little relevance to radionuclide transport from a deep repository, and can be neglected by assuming steady-state flow conditions for nominal natural system analysis. At longer time scales the groundwater flow conditions may be altered by climate change, anthropogenic influences via groundwater pumping, and geomorphic evolution (at very long time scales). Analysis of disturbed scenarios for changes to the groundwater flow system is often determined by policy and regulatory decisions. Generally, the impacts on groundwater flow of disturbed conditions can be evaluated by changing the boundary conditions of the nominal-case model and allowing transient changes to propagate through the system.

The natural system would also experience transient conditions for heat flow and mechanical stress due to the presence of the repository. Temperature perturbations may extend for significant distances from the repository into the natural system and persist for hundreds or thousands of years; however, the magnitude of change in temperature declines rapidly with distance from the repository. Mechanical effects may also impact the natural system, but have significant impacts only very near the repository. Coupled thermal-hydrologic processes can produce transient groundwater flow conditions in the natural system, but have limited impact on groundwater flow and radionuclide transport for the three mined repository systems. For the deep borehole disposal concept coupled thermal-hydrologic flow would be the primary process driving fluid flow and radionuclide transport for a deep hydrogeological system that lacks significant ambient gradients in fluid potential.

5. NUMERICAL IMPLEMENTATION AND ARCHITECTURE

As described in Section 1.2, the generic natural system model must be flexible, well integrated with the GDSM, and numerically efficient. The numerical implementation and architecture of the model should be designed to help support these requirements. Numerous options for numerical implementation exist and selection of appropriate methods often involves tradeoffs among competing modeling requirements. In this sense, hybrid or combined numerical implementation options are often the best compromise.

5.1 Review of Numerical Implementation Options

Several numerical methods using spatial discretization or gridding of the problem domain are commonly used in numerical models of groundwater flow, solute transport, heat transport, and solid mechanics. These methods include finite difference, finite element, finite volume, and integrated finite difference techniques. These methods use an Eulerian frame of reference in which flow and transport are analyzed from a spatially rigid perspective. Alternatively, flow and transport can be analyzed from a Lagrangian frame of reference in which individual parcels of fluid or solute mass are tracked through space. The Lagrangian approach can be advantageous in simulating solute transport in groundwater flow systems, as a particle tracking algorithm.

Eulerian numerical methods like the finite element method are very successful for simulating generally highly diffusive properties of the natural system such as fluid pressure in groundwater flow, temperature in heat transport, and stress in solid mechanics, particularly in homogeneous or mildly heterogeneous media. The grid resolution and the associated computational burden required to accurately model these processes is related to the magnitude of the gradients in the dependent properties and the degree of heterogeneity in the media. As examples, the grid resolution near a pumping well must be higher to accurately represent the gradient in hydraulic head and the grid resolution near the EBS must be higher to accurately simulate the gradients in temperature associated with repository heat. A moderate amount of heterogeneity in permeability within the medium can be accurately represented with a uniform grid; however, highly heterogeneous media and explicit representation of discrete fractures require extremely high grid resolution in the strictly Eulerian approach.

For solute transport in systems that are advectively dominated, strictly Eulerian numerical methods are much less successful. Very high grid resolution, particularly at the front of an advancing solute plume is required to obtain an accurate numerical solution. This is because numerical dispersion inherent in Eulerian methods overwhelms physical dispersion, leading to “smearing” of the simulated solute plume and unrealistically low simulated solute concentrations. Solute mass balance errors can also be a problem in Eulerian methods.

Lagrangian numerical methods have the advantage in solute transport simulations of limited numerical dispersion that is generally independent of grid resolution (e.g., see Zheng, 1990). Often implemented as a particle tracking method, the Lagrangian approach also enforces solute mass balance in solute transport modeling. In addition, Lagrangian numerical methods are numerically much more efficient than Eulerian methods for solute transport.

Hybrid methods that combine the respective strengths of the Eulerian and Lagrangian numerical approaches can be used to model the natural system for performance assessment analyses. Three-dimensional Eulerian modeling of groundwater flow, thermal processes, and mechanics would be used in combination with particle tracking to define paths for radionuclide transport through the generic natural system model. Essentially one-dimensional modeling would then be used to simulated radionuclide transport from the EBS to the biosphere. The one-dimensional modeling of transport can be directly coupled to the three-dimensional modeling of other processes to capture transient effects in flow and heat transport or time-invariant flow paths can be extracted for simplified, decoupled simulation of radionuclide transport. Examples of numerical methods using hybrid approaches that are relevant to nuclear waste disposal and natural system modeling include Arnold et al. (2003), Robinson et al. (2010), and Painter et al. (2008).

Furthermore, numerical methods applied to numerical models of groundwater flow, solute transport, heat transport, and solid mechanics are dependent on the conceptual simplifications applied to the media in the natural system. These alternative implementation methods of conceptual flow models are summarized in Altman et al. (1996), as shown in Figure 5-1 and include the following alternatives, listed from least to most complex:

- Equivalent Porous Medium Continuum – All processes and material properties treated as a porous medium in a single continuum. Equivalent material properties are based on effective characteristics of the medium.
- Composite Porosity Continuum - All processes and material properties treated as a porous medium in a single continuum. Some material properties (e.g., relative permeability – capillary pressure relationships) are altered to reflect the effects of fractures.
- Dual Porosity – Processes and materials are represented by two collocated continua, the fracture continuum and the matrix continuum. Flow occurs only in the fracture continuum, but fluid and solute exchange occurs between the fracture continuum and the matrix continuum.
- Dual Permeability - Processes and materials are represented by two collocated continua, the fracture continuum and the matrix continuum. Flow occurs both in the fracture continuum and in the matrix continuum. Fluid and solute exchange also occur between the fracture continuum and the matrix continuum.
- Discrete Fracture Network – Individual fractures are discretely represented. Flow and transport only occur in the fractures.
- Discrete Fracture Network with Matrix - Individual fractures are discretely represented. Flow and transport occur in both the fractures and matrix. Fluid and solute exchange also occur between the fractures and the matrix.

Different alternative implementation methods may be appropriate for different units within the generic natural system model and for different disposal system alternatives. The equivalent porous medium approach is valid for aquifers consisting of granular media and probably for low-permeability host rock such as clay. The dual-porosity approach is appropriate for densely fractured units, such as fractured carbonate aquifers and for fractured crystalline rock as some sites. The discrete fracture network with matrix approach may be required for granite host rock at some sites.

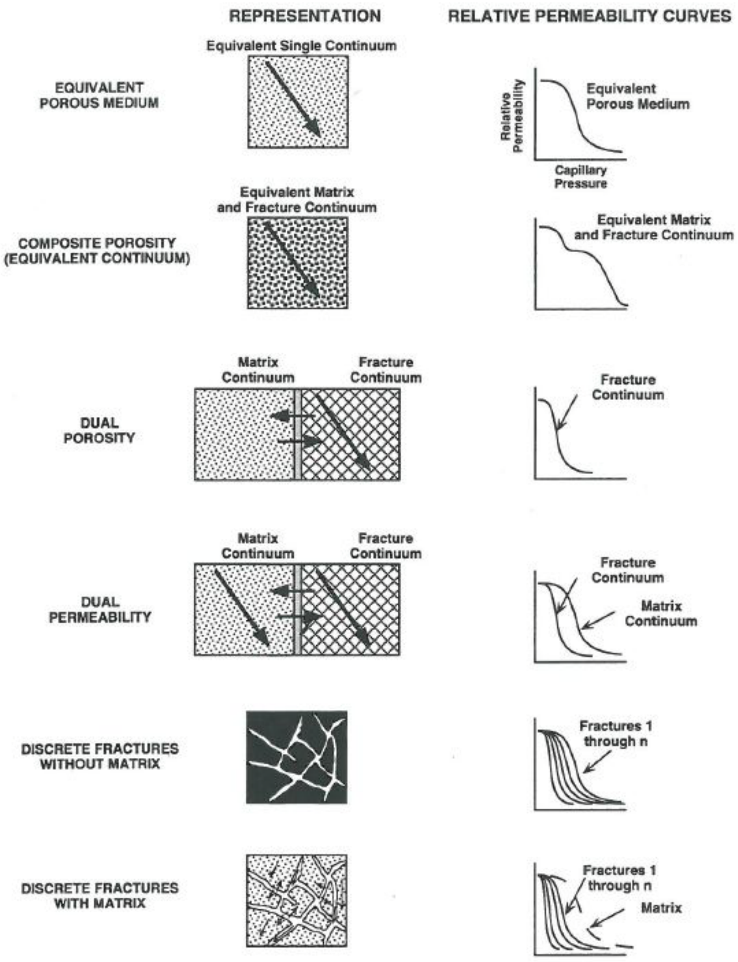


Figure 5-1. Alternative Implementation Methods of Conceptual Flow Models (from Altman et al., 1996).

The appropriate implementation method may also be a function of spatial scale. For example, radionuclide transport of a few hundred meters through fractured crystalline rock from a mined repository may require a discrete fracture network approach, whereas transport of a few thousand meters through fractured crystalline rock from deep borehole disposal might appropriately use a continuum dual-porosity approach. Computationally efficient methods have also been developed that effectively upscale solute transport behavior in discrete fracture networks for implementation with a continuum approach (e.g., Painter and Cvetkovic, 2005).

5.2 Selection of Numerical Implementation Methods

Based on the discussion presented in the previous section, the recommended approach for numerical implementation of the generic natural system model would use a hybrid numerical method. The processes of groundwater flow, heat transport, and mechanics would be simulated using a three-dimensional model based on Eulerian methods. Heat transport and mechanics can be accommodated using a continuum representation for all units in the natural system.

Groundwater flow may be simulated using the equivalent porous medium representation for some units, but may require a dual-porosity, dual-permeability, or discrete fracture representation in other units. Large-scale discrete fracture network representations with matrix participation for the entire natural system model are generally beyond the computational reach of standard finite-element formulations. However, advanced finite-element gridding methods to explicitly include discrete fracture networks at large scales are under development.

The processes associated with radionuclide transport would be based on Lagrangian methods. These would be applied along essentially one-dimensional pathways through the generic natural system model using multiple stochastically generated particle tracks representing packets of radionuclide mass. The one-dimensional nature of the solute transport solution would be computationally efficient and could accommodate full simulation of radionuclide decay chains.

Numerical solution techniques that are appropriate for local conditions could be applied to different segments of the transport pathway through the system to improve computational efficiency. Such an approach is illustrated in Figures 5-2 and 5-3. Figure 5-2 shows a schematic representation of the flow path for a given parcel of radionuclide mass derived from the full three-dimensional generic natural system model. In this example, the flow path includes segments that are dominated by diffusion, as in the clay host rock, and segments that are dominated by advective groundwater flow, as in the two aquifers overlying the host rock.

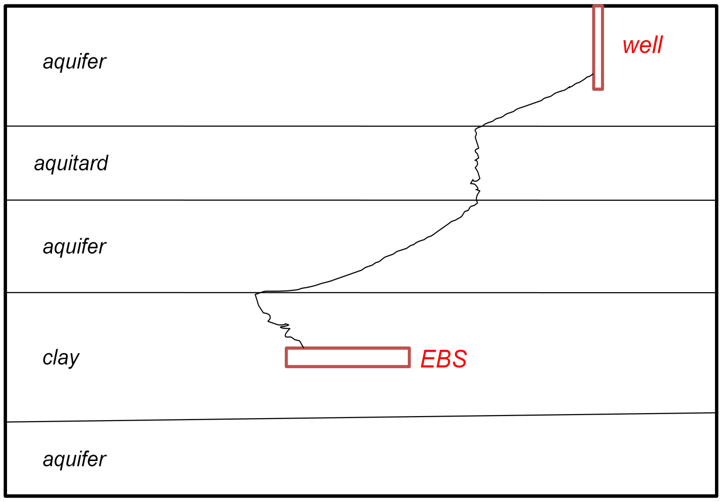


Figure 5-2. Schematic Hydrogeologic Framework and Particle Path in the Natural System

The contribution of advective solute transport relative to dispersive or diffusive transport at any point along the flow path can be evaluated using the dimensionless Péclet number. The Péclet number for longitudinal flow and transport is given by:

$$\boldsymbol{Pe_L = \frac{v_L L}{D_\alpha^e}} \tag{5-1}$$

where *L* is the characteristic length in the longitudinal direction and generally taken as the grid resolution for evaluating the Péclet number in a numerical model. Figure 5-3 shows the value of the Péclet number calculated as a function of distance along the flow path.

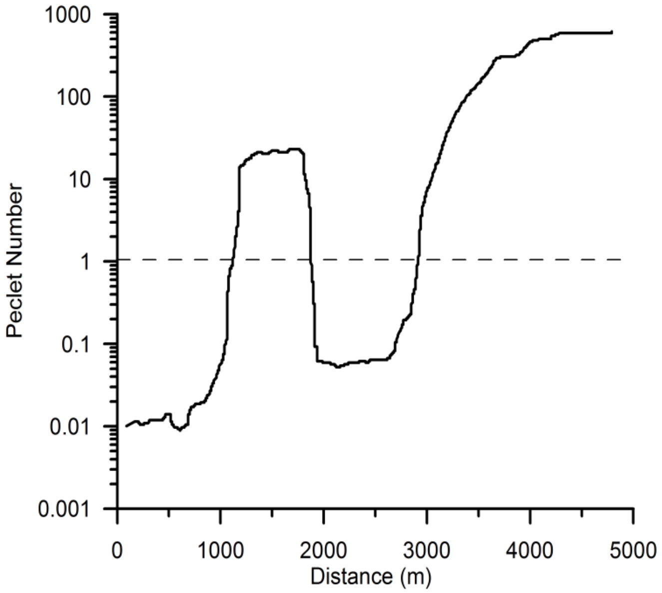


Figure 5-3. Diagrammatic Plot of Péclet Number Versus Distance Along Particle Path in the Natural System.

For those portions of the flow path in which diffusion dominates (e.g., Péclet number of less than 0.1), a simplified equivalent porous medium, diffusion-only solution would be implemented. For locations along the particle path in which groundwater flow dominates transport, an advection-dispersion solution would be applied, with potentially dual-porosity mass transfer applied in fractured units.

5.3 Preliminary Numerical Architecture and Interface with GDSM

The preliminary recommended numerical architecture for the generic natural system model is described in this section. The model will be a three-dimensional model for the processes of groundwater flow, heat transport, and solid mechanics. The internal structure of the generic natural system model will consist of simplified, but reasonable representations of hydrogeologic units, specific to each disposal system, as shown in Table 4-1. The dimensions and boundary conditions of the generic natural system model are the same for the three mined repository concepts, and are different for the deep borehole disposal concept. The option will exist to turn off the heat transport and mechanics processes in the model, which may be acceptable for many GDSM applications, and will lead to significantly greater computational efficiency. An additional option will allow the groundwater flow solution to be “frozen” under steady-state conditions. Radionuclide transport will be simulated along one-dimensional flow paths that have been determined using particle tracking methods in the three-dimensional model. Radionuclide transport modeling will include the processes of advection, dispersion, diffusion, sorption, matrix diffusion in fractured media, and colloid-facilitated transport. Simulations will include all members of decay chains.

The generic natural system model will consist of a stand-alone numerical model that will be executed in parallel to the GDSM. Time stepping will be controlled by the overall GDSM, with shorter time step looping occurring in the generic natural system model by controlling numerical factors within the natural system model. Input to the generic natural system model from the EBS component of the GDSM will include radionuclide mass release from the EBS, thermal output, and mechanical stress. As noted above, the inputs of thermal output and mechanical stress would be disabled for simulations that do not include heat transport and solid mechanics. Other inputs from the GDSM may include initiating events that would change the boundary conditions or material properties within the natural system, such as climate change, seismic events, or continental glaciations. Output of the generic natural system model to the biosphere component will be radionuclide mass release for each GDSM time step.

For the preliminary generic natural system model simplifying assumptions about interfaces with other components of the GDSM will be applied. The interface between the generic natural system model and the EBS will be represented as a rectangular prism, with homogenized or “smeared” sources of radionuclide mass, heat, and stress within the natural system. The interface with the biosphere will be a continuously pumping hypothetical well, in which the radionuclide concentrations in the well water will be calculated using the radionuclide release rate and the pumping rate of the well.

6. SUMMARY AND CONCLUSIONS

The conceptual model and numerical architecture of the generic natural system model have been evaluated and described with the objectives of: 1) reviewing FEPs relevant to the four alternative disposal systems, 2) identification of associated mathematical models, 3) articulation of reference conceptual models, 4) exploration of alternative strategies for numerical implementation, and 5) defining a treatment of FEPs, conceptual models, and interfaces that is consistent with other components of the GDSM. These objectives for the generic natural system model were met based on the basic requirements that the model be inclusive, comprehensive, flexible, integrated with other GDSM components, and numerically efficient.

A list of 51 FEPs applicable to the natural system identified by Freeze et al. (2010) was used as the starting point for an evaluation of FEPs in the generic natural system model. The evaluation encompassed the four alternative disposal systems and four potential waste types. Previous work on the prioritization of FEPs documented in DOE (2011) was considered in the evaluation. These evaluations resulted in the retention of 35 FEPs and the exclusion of 16 FEPs in the generic natural system model. Details of the screening and prioritization results are shown in Table A-1. Results also show that many FEPs have relatively low overall priority with regard to research and development, but vary significantly in importance to the safety case. FEPs for the salt repository, clay repository, and deep borehole disposal concepts generally have higher priority scores than FEPs for the granite repository concept.

A comprehensive set of general mathematical models for the FEPs in the generic natural system model is presented in Section 3. Mathematical terms in many of these governing equations are not necessarily needed for some of the FEPs, disposal concepts, or individual hydrogeologic units in the generic natural system model, but are included for completeness. For example, relative permeability and capillary pressure terms and relationships are only relevant to multiphase fluid flow and are thus unnecessary in saturated units in the model. Alternative mathematical models for a single process, such as sorption, are also presented in the list of mathematical models.

A conceptual model for the generic natural system model is presented in Section 4. Specific components of the conceptual model for the four alternative disposal systems are summarized in Table 4-1. This conceptual model consists of a three-dimensional domain, with variations in hydrogeologic framework, boundary conditions, and domain dimensions for the alternative disposal systems. Potential release scenarios, alternative representations of interfaces with the EBS and biosphere, and transience in the natural system are also discussed. The spatial resolution or complexity of the interfaces with the EBS and biosphere may be constrained by computational feasibility and regulatory assumptions.

Options for the numerical implementation of the conceptual and mathematical models are examined in a general sense in Section 5, with particular emphasis on differences between Eulerian and Lagrangian numerical methods. Eulerian approaches, such as the finite-element method are appropriate for moderately to highly diffusive processes such as groundwater flow, heat transport, and solid mechanics. Lagrangian approaches, such as particle tracking are more accurate and numerically efficient for advectively dominated solute transport, particularly in highly heterogeneous or fractured media. The recommended approach for numerical implementation of the generic natural system model would use a hybrid numerical method. The processes of groundwater flow, heat transport, and mechanics would be simulated using a three-dimensional model based on Eulerian methods. The processes associated with radionuclide transport would be based on Lagrangian methods and would be applied along essentially one-dimensional pathways through the generic natural system model using multiple stochastically generated particle tracks representing packets of radionuclide mass. The generic natural system model will consist of a stand-alone numerical model that will be executed in parallel to the GDSM. Potential inputs to the generic natural system model from the EBS component of the GDSM will include radionuclide mass release from the EBS, thermal output, and mechanical stress. Output of the generic natural system model to the biosphere component will be radionuclide mass release for each GDSM time step.

It should be noted that the conclusions documented in this report regarding the generic natural system model are preliminary. Actual implementation of the model would be subject to the availability and limitations of software codes capable of the computations involved in the recommended numerical implementation. Structuring the interfaces with the GDSM and implementation of the recommended approach are feasible, but would involve considerable technical development and effort.

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Appendix A

FEP Screening and Mapping to Geosphere Components

This appendix provides the summary of mapping natural systems (geosphere) FEPs and associated processes to the different geosphere components and sub-components for the different disposal concepts/geologic settings described in details in Section 2.2. The summary is presented in Table A-1.

Table A-1 contains the number, the name, and the associated processes for each of all 51 natural systems FEPs. Each process is either considered to be applicable or not applicable. The not-applicable processes also include the processes excluded based on low importance/low consequences. The not-applicable/excluded FEPs are not marked.

The applicable processes are categorized either as "very important" or "somewhat important". The very important processes are those that need to be implemented in the generic natural system conceptual model. The importance is defined based on the capability of the process to facilitate or delay radionuclide transport and/or to enhance or diminish the component performance. The somewhat important processes may or may not be implemented in the generic natural system conceptual model. The applicable processes are marked with "**x**". The very important processes are shown in red font. The somewhat important processes are shown in blue font.

The applicability/importance of each process is shown for each component and sub-component of geosphere. As discussed in Section 2.1, the geosphere components are: EDZ, Host Rock, and Other Units. The sub-components of EDZ and Host Rock are: Granite, Clay, Salt, and Deep Borehole. The sub-components of the Other Units are: Confining Units, Aquifer, and Unsaturated Units.

Some geosphere FEPs are closely related to the other geosphere FEPs or/and to the EBS, Biosphere, and External FEPs. If this is the case, the names and the numbers of the related FEPs are shown for each applicable process in the following columns of Table A-1 as appropriate: "Related FEPs in Geosphere"; "Related FEPs in EBS"; "Related FEPs in Biosphere"; and Related FEPs in External".

Additional information in Table A-1 includes the results of YMP screening from the YMP FEPs list (SNL 2008). These results are in column "YMP Screening". Note that YMP screening applies to a FEP and does not differentiate between the processes included in the FEP. The FEP is either "Excluded" or "Included".

Five columns under the "UFD Roadmap Evaluation" in Table A-1 contain the safety case importance scores (IS_a, IS_d, and IS_c, and IS) and overall priority scores (P). The values for the importance to the safety case components IS_a, IS_d, and IS_c were taken from appendix A in (DOE, 2011). These values are either 1 (low importance), or 2 (medium importance), or 3 (high importance). The resulting importance to safety case (IS) values were calculated as described in

Section 2.1 using Equation 2-1, decision point specific weights $w_{a,k}$ from Table 2 in (DOE, 2011), and the decision point specific weights α_k from Table 5 in (DOE, 2011).

The overall priority scores P are from Appendix B in (DOE, 2011). Note that in a number of cases P is disposal concept specific. The values of P change from 0 to 13.

As explained in Section 2.1, the importance to the safety case scores and overall priority scores are provided to assist in screening decision. In general, the included FEPs are also the ones with high importance to the safety case (but not necessarily with the high priority) with a few exceptions. The excluded FEPs are also the ones with low importance to the safety case (but not necessarily with the low priority) with a few exceptions. The excluded FEPs are specifically summarized in Table 2-1.

A-1. Summary Table

Table A-1. Summary of Natural Systems FEPs Evaluation.

Table A-1. Summary of Natural Systems FEPs Evaluation

NN	YMP Screening Results	FEP NN	FEP Name	FEP Processes	UFD Roadmap Evaluation								EDZ				Host Rock				Other Units			Related FEPs			
					Importance to Safety Case Scores				Overall Priority Scores (*P*)																		
					IS_a	IS_d	IS_c	IS	Granite	Clay	Salt	Borehole	Granite	Clay	Salt	Borehole	Granite	Clay	Salt	Borehole	Confining Units	Aquifer	Unsaturated Units	Geosphere	EBS	Biosphere	External
		2.2.01.00	**EXCAVATION DISTURBED ZONE (EDZ)**																								
1	Excluded	**2.2.01.01**	**Evolution of EDZ**		3	3	3	**3**	2.58	8	2.58	6.13															
				Lateral extent, heterogeneities									x	x	x	x											Mechanical Effects of Excavation in 1.1.02.02
				Physical properties									x	x	x	x											
				Flow pathways									x	x	x	x											
				Chemical characteristics of groundwater in EDZ																							
				Radionuclide speciation and solubility in EDZ																							
				Thermal-mechanical effects												x											
				Thermal-chemical alteration																							
		2.2.02.00	**HOST ROCK**																								
2	Included	**2.2.02.01**	**Stratigraphy and Properties of Host Rock**		3	2	3	**2.8**	3.74	3.74	3.74	3.74															
				Rock units													x	x	x	x				Fractures in 2.2.05.01			
				Thickness, lateral extent, heterogeneities, discontinuities, contacts													x	x	x	x				Faults in 2.2.05.02			
				Physical properties													x	x	x	x							
				Flow pathways													x	x	x	x							
		2.2.03.00	**OTHER GEOLOGIC UNITS**																								
3	Included	2.2.03.01	**Stratigraphy and Properties of Other Geologic Units (Non-Host-Rock)**		3	1	3	**2.6**	2.46	2.46	2.46	2.46															
				Rock units																	x	x	x	Fractures in 2.2.05.01			
				Thickness, lateral extent, heterogeneities, discontinuities, contacts																	x	x	x	Faults in 2.2.05.02			
				Physical properties																	x	x	x				
				Flow pathways																	x	x	x				
		2.2.05.00	**FLOW AND TRANSPORT PATHWAYS (Host Rocks and Other Geologic Units)**																								
4	Included	2.2.05.01	**Fractures**		3	1	3	**2.6**	3.65	3.65	3.65	3.65															
				Rock properties													x	x	x	x	x	x	x	Stratigraphy and Properties, 2.2.02.01			
5	Included	2.2.05.02	**Faults**		N/A	N/A	N/A	**N/A**	N/A	N/A	N/A	N/A															
				Rock properties													x	x	x	x	x	x	x	Stratigraphy and Properties, 2.2.03.01			
6	N/A	2.2.05.03	**Alteration and Evolution of Geosphere Flow Pathways**		1	N/A	1	**1**	2.46	2.46	2.46	2.46															
				Changes In rock properties													x	x	x	x				Stratigraphy and Properties in 2.2.02.01 and			1.1.02.03 “Thermal-Hydrologic

			Changes in faults															2.2.03.01 Thermal-Mechanical Effects in 2.2.11.06 Fractures in 2.2.05.01 Faults in 2.2.05.02 Thermal-Chemical Alteration in 2.2.11.07		Effects from Preclosure Operations 1.1.02.02 “Mechanical Effects from Preclosure Operations”
			Changes in fractures										x	x	x	x				
			Plugging of flow pathways																	
			Changes in saturation														x			
		2.2.07.00	**MECHANICAL PROCESSES**																	
7	Excluded	2.2.07.01	**Mechanical Effects on Host Rock**	3	3	3	**3**	1.63	3.83	3.83	1.63							Subsidence in 1.2.02.01 Thermal-Mechanical Effects in 2.2.11.06 Thermal-Chemical Alteration in 2.2.11.07		
			From subsidence																	
			From salt creep												x					
			From clay deformation											x						
			From granite deformation (rockfall / drift collapse into tunnels)										x							
			Chemical precipitation /dissolution																	
			Stress regimes													x				
8	Excluded	2.2.07.02	**Mechanical Effects on Other Geologic Units**	2	N/A	2	**2**	1.32	3.1	3.1	1.32							Thermal-Chemical Alteration in 2.2.11.07 Thermal-Mechanical Effects in 2.2.11.06		Subsidence in 1.2.02.01
			From subsidence																	
			Chemical precipitation /dissolution																	
			Stress regimes																	
		2.2.08.00	**HYDROLOGIC PROCESSES**																	
9	Included	2.2.08.01	**Flow through the Host Rock**	3	1	3	**2.6**	0	3.65	7.73	3.65							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	Influx/Seepage into EBS in 2.1.08.09	
			Saturated flow										x	x	x	x				
			Fracture flow / matrix imbibition										x	x	x	x				
			Unsaturated flow (fingering, capillarity, episodicity, perched water)																	
			Preferential flow pathways										x	x	x	x				
			Density effects on flow																	
			Flow pathways out of Host Rock										x	x	x	x				
10	Included	2.2.08.02	**Flow through the Other Geologic Units**	3	1	3	**2.6**	0	3.65	7.73	3.65									

			Saturated flow															x	x		Alteration of Flow Pathways in 2.2.05.03, Thermal Effects on Flow in 2.2.11.01,		
			Fracture flow / matrix imbibition															x	x				
			Unsaturated flow (fingering, capillarity, episodicity, perched water)																		Effects of Gas on Flow in 2.2.12.02		
			Preferential flow pathways															x					
			Density effects on flow																				
			Flow pathways out of Other Geologic Units															x	x	x			
11	Incl/Excl	2.2.08.03	**Effects of Recharge on Geosphere Flow (Host Rocks and Other Geologic Units)**	N/A	N/A	N/A	**N/A**	0	0	0	0												
			Infiltration rate															x	x	x			Infiltration in 2.3.08.03
			Water table rise/decline															x	x	x			
12	Incl/Excl	2.2.08.04	**Effects of Repository Excavation on Flow through the Host Rock**	2	1	2	**1.8**	0	3.23	7.1	3.23											Influx/Seepage into EBS in 2.1.08.09	
			Saturated flow (flow sink)												x	x	x						
			Unsaturated flow (capillary diversion, drift shadow)																				
			Influx/Seepage into EBS (film flow, enhanced seepage)																				
13	Excluded	2.2.08.05	**Condensation Forms in Host Rock**	N/A	N/A	N/A	**N/A**	0	0	0	0												
			Condensation cap																		Thermal Effects on Flow in Geosphere in 2.2.11.01		
			Shedding																				
14	Excluded	2.2.08.06	**Flow through EDZ**	3	1	3	**2.6**	0	3.65	7.73	3.65												
			Saturated / Unsaturated flow									x	x	x									
			Fracture / Matrix flow									x	x	x									
15	Excluded	2.2.08.07	**Mineralogic Dehydration**	1	2	1	**1.2**	0	2.82	6.49	2.82												
			Dehydration reactions release water and may lead to volume changes																				
16	Excluded	2.2.08.08	**Groundwater Discharge to Biosphere Boundary**	N/A	N/A	N/A	**N/A**	0	0	0	0												
			Surface discharge (water table, capillary rise, surface water)															x	x	x			
			Flow across regulatory boundary															x	x	x			
17	Included	2.2.08.09	**Groundwater Discharge to Well**	N/A	N/A	N/A	**N/A**	0	0	0	0												
			Human use (drinking water, bathing water, industrial)																x	x			
			Agricultural use (irrigation, animal watering)																x	x			
		2.2.09.00	**CHEMICAL PROCESSES - CHEMISTRY**																				
18	Included	2.2.09.01	**Chemical Characteristics of**	3	N/A	3	**3**	0	3.55	2.4	5.86												

			Groundwater in Host Rock																					
			Water composition (radionuclides, dissolved species, …)									x	x	x	x	x	x	x	x				Chemical Interactions and Evolution in 2.2.09.03	Chemistry in Tunnels in 2.1.09.04
			Water chemistry (temperature, pH, Eh, ionic strength …)									x	x	x	x	x	x	x	x					Chemistry of Water Flowing into Repository in 2.1.09.01
			Reduction-oxidation potential									x	x	x	x	x	x	x	x					
			Reaction kinetics									x	x	x	x	x	x	x	x					
			Interaction with EBS									x	x	x	x	x	x	x	x					
			Interaction with host rock									x	x	x	x	x	x	x	x					
19	Included	2.2.09.02	**Chemical Characteristics of Groundwater in Other Geologic Units**	3	N/A	3	3	0	3.55	2.4	5.86													
			Water composition (radionuclides, dissolved species, …)																	x	x	x	Chemical Interactions and Evolution in 2.2.09.03	
			Water chemistry (temperature, pH, Eh, ionic strength …)																	x	x	x		
			Reduction-oxidation potential																	x	x	x		
			Reaction kinetics																	x	x	x		
			Interaction with other geologic units																	x	x	x		
20	Excluded	2.2.09.03	**Chemical Interactions and Evolution of Groundwater in Host Rock**	2	N/A	2	2	0	3.1	2.1	5.4													
			Host rock composition and evolution (granite, clay, salt ...)																				Chemistry in Host Rock in 2.2.09.01	
			Evolution of water chemistry in host rock																	`				
			Chemical effects on density																					
			Interaction with EBS									x	x	x	x	x	x	x	x					
			Reaction kinetics																					
			Mineral dissolution/precipitation																					
			Redissolution of precipitates after dry-out																					
21	Excluded	2.2.09.04	**Chemical Interactions and Evolution of Groundwater in Other Geologic Units**	2	N/A	2	2	0	3.1	2.1	5.4													
			Host rock composition and evolution (granite, clay, salt ...)																				Chemistry in Other Geologic Units in 2.2.09.02	
			Evolution of water chemistry in host rock																					
			Chemical effects on density																					
			Reaction kinetics																					
			Mineral dissolution/precipitation																					
			Recharge chemistry																					
22	Excluded	2.2.09.05	**Radionuclide Speciation and Solubility in Host Rock**	3	N/A	3	3	0	3.55	2.4	5.86													
			Dissolved concentration limits																				Chemistry in Host Rock in	

23	Excluded	2.2.09.06	**Radionuclide Speciation and Solubility in Other Geologic Units**	3	N/A	3	3	0	3.55	2.4	5.86								2.2.09.01
			Dissolved concentration limits																Chemistry in Other Geologic Units in 2.2.09.02
		2.2.09.50	**CHEMICAL PROCESSES - TRANSPORT**																
24	Included	2.2.09.51	**Advection of Dissolved Radionuclides in Host Rock**	3	2	3	2.8	3.74	3.74	2.53	2.53								
			Flow pathways and velocity									x	x		x				Gas Phase Transport in 2.2.12.0
			Advective properties (porosity, tortuosity)									x	x		x				
			Dispersion									x	x		x				
			Matrix diffusion									x	x		x				
			Saturation																
25	Included	2.2.09.52	**Advection of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock)**	3	2	3	2.8	3.55	33.55	2.4	2.4								
			Flow pathways and velocity													x	x		Gas Phase Transport in 2.2.12.0
			Advective properties (porosity, tortuosity)													x	x		
			Dispersion													x	x		
			Matrix diffusion													x	x		
			Saturation																
26	Included	2.2.09.53	**Diffusion of Dissolved Radionuclides in Host Rock**	3	N/A	3	3	3.55	33.55	2.4	2.4								
			Gradients (concentration, chemical potential)									x	x	x	x				
			Diffusive properties (diffusion coefficients)									x	x	x	x				
			Flow pathways and velocity									x	x	x	x				
			Saturation																
27	Included	2.2.09.54	**Diffusion of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock)**	3	N/A	3	3	3.55	33.55	2.4	2.4								
			Gradients (concentration, chemical potential)											`		x	x		
			Diffusive properties (diffusion coefficients)													x	x		
			Flow pathways and velocity													x	x		
			Saturation																
28	Included	2.2.09.55	**Sorption of Dissolved Radionuclides in Host Rock**	3	N/A	3	3	3.55	33.55	2.4	2.4								
			Surface complexation properties									x	x	x	x				Chemistry in Host Rock in 2.2.09.01
			Flow pathways and velocity									x	x	x	x				
			Saturation																
29	Included	2.2.09.56	**Sorption of Dissolved Radionuclides in Other Geologic Units**	3	N/A	3	3	3.55	33.55	2.4	2.4								
			Surface complexation properties													x	x	x	Chemistry in Other Geologic Units in 2.2.09.02

			Flow pathways and velocity																	x	x	x	
			Saturation																			x	
30	Included	2.2.09.57	**Complexation in Host Rock**	3	N/A	3	**3**	3.55	33.55	2.4	2.4												
			Presence of organic complexants (humates, fulvates, carbonates, …)									x	x	x	x	x	x	x	x				Radionuclide Speciation in 2.2.09.06 for inorganic complexation
			Enhanced transport of radionuclides associated with organic complexants									x	x	x	x	x	x	x	x				
31	Included	2.2.09.58	**Complexation in Other Geologic Units (Non-Host-Rock**	3	N/A	3	**3**	3.55	33.55	2.4	2.4												
			Presence of organic complexants (humates, fulvates, carbonates, …)																	x	x	x	
			Enhanced transport of radionuclides associated with organic complexants																	x	x	x	
32	Included	2.2.09.59	**Colloidal Transport in Host Rock**	2	N/A	3	**2.38**	3.29	3.29	2.22	2.22												
			Flow pathways and velocity									x	x	x	x	x	x	x	x				
			Saturation																				
			Advection									x			x	x			x				
			Dispersion									x			x	x			x				
			Diffusion									x	x	x	x	x	x	x	x				
			Sorption									x	x	x	x	x	x	x	x				
			Colloid concentration									x	x	x	x	x	x	x	x				
33	Included	2.2.09.60	**Colloidal Transport in Other Geologic Units**	2	N/A	3	**2.38**	3.29	3.29	2.22	2.22												
			Flow pathways and velocity																	x	x		
			Saturation																				
			Advection																		x		
			Dispersion																		x		
			Diffusion																	x	x		
			Sorption																	x	x		
			Colloid concentration																	x	x		
34	Excluded	2.2.09.61	**Radionuclide Transport Through EDZ**	3	N/A	3	**3**	3.55	3.55	2.4	2.4												
			Advection									x	x		x								
			Dispersion									x	x		x								
			Diffusion					`				x	x	x	x								
			Sorption									x	x	x	x								
35	Included	2.2.09.62	**Dilution of Radionuclides in Groundwater (Host Rocks and Other Geologic Units)**	2	N/A	2	**2**	3.1	3.1	2.1	2.1												
			Mixing with uncontaminated groundwater																		x		Groundwater Discharge to Well in 2.2.08.09
			Mixing at withdrawal well																		x		
36	Excluded	2.2.09.63	**Dilution of Radionuclides with Stable Isotopes (Host Rocks and Other Geologic Unuts)**	2	N/A	2	**2**	3.1	3.1	2.1	2.1												
			Mixing with stable and/or naturally occurring isotopes of the same element																				

37	Inc/Exc	2.2.09.64		**Radionuclide Release from Host Rock**	3	N/A	3	3	3.5	3.5	2.4	2.4											
			Dissolved	Releases to the Other Geologic Units or Biosphere											x	x	x	x				Dissolved in 2.2.09.51/53/55	
			Colloidal																			Colloidal in 2.2.09.59	
			Gas Phase																			Gas Phase in 2.2.12.03	
																						EDZ in 2.2.09.61	
38	Inc/Exc	2.2.09.65		**Radionuclide Release from Other Geologic Units**	3	N/A	3	3	3.5	3.5	2.4	2.4											
			Dissolved	Releases to the Other Geologic Units or Biosphere															x	x	x	Dissolved in 2.2.09.52/54/56	Recycling of Accumulated Radionuclides in 2.3.09.55
			Colloidal																			Colloidal in 2.2.09.60	
			Gas Phase																			Gas Phase in 2.2.12.03 Groundwater Discharge to Biosphere Boundary in 2.2.08.08, Groundwater Discharge to Well in 2.2.08.09	
		2.2.10.00	**BIOLOGICAL PROCESSES**																				
39	Excluded	2.2.10.01		**Microbial Activity in Host Rock**	2	N/A	2	2	1.32	1.32	1.32	1.32											
				Formation of complexants																		Complexation in Host Rock in 2.2.09.57	
				Formation and stability of microbial colloids																			
				Biodegradation																			
				Bioaccumulation																			
40	Excluded	2.2.10.02		**Microbial Activity in Other Geologic Units (Non-Host-Rock)**	2	N/A	2	2	1.32	1.32	1.32	1.32											
			Confining units	Formation of complexants																		Complexation in Other Geologic Units in 2.2.09.58	
			Aquifers	Formation and stability of microbial colloids																			
				Biodegradation																			
				Bioaccumulation																			
		2.2.11.00	**THERMAL PROCESSES**																				
41		2.2.11.01		**Thermal Effects on Flow in Geosphere**	2	N/A	2	2	2.1	3.1	2.1	3.1											
	Excluded			Altered gradients, density, and/or flow pathways									x	x	x			x					
	Excluded			Condensation																			
	Excluded			Vapor flow																			
	Included			Condensation																			
42	Excluded	2.2.11.02		**Thermally-Driven Flow (Convection) in Geosphere**	2	N/A	2	2	2.1	3.1	2.1	3.1											
				Convection									x	x	x			x					
43	Included	2.2.11.03		**Thermally-Driven Buoyant Flow / Heat Pipes in Geosphere**	1	N/A	1	1	1.66	2.46	1.66	2.46											
				Vapor Flow																			
44	Excluded	2.2.11.04		**Thermal Effects on Chemistry and**	3	N/A	3	3	2.4	3.55	2.4	3.55											

			Microbial Activity in Geosphere Mineral precipitation / dissolution Altered solubility																Chemistry in 2.2.09.01 and 2.2.09.02
45	Excluded	2.2.11.05	**Thermal Effects on Transport in Geosphere** Thermal diffusion (Soret effect) Thermal osmosis	N/A	N/A	N/A	**N/A**	0	0	0	0								
46	Excluded	2.2.11.06	**Thermal-Mechanical Effects on Geosphere** Thermal expansion / compression Altered properties of fractures, faults, rock matrix	2	1	3	**2.38**	2.3	3.4	2.3	3.4			x			x		
47	Excluded	2.2.11.07	**Thermal-Chemical Alteration of Geosphere** Mineral precipitation / dissolution Altered properties of fractures, faults, rock matrix Alteration of minerals / volume changes Formation of near-field chemically Altered zone (rind)	2	1	3	**2.38**	2.3	3.4	2.3	3.4								
		2.2.12.00	**GAS SOURCES AND EFFECTS**																
48	Excluded	2.2.12.01	**Gas Generation in Geosphere** Degassing (clathrates, deep gases) Microbial degradation of organics Vaporization of water	N/A	N/A	N/A	**N/A**	0	0	0	0								
49	Excluded	2.2.12.02	**Effects of Gas on Flow Through the Geosphere** Altered gradients and/or flow pathways Vapor/air flow Two-phase flow Gas bubbles	2	1	2	**2**	0.95	0.95	0.95	0.95	x	x		x	x			Buoyant Flow/Heat Pipes in 2.2.11.03
50	Excluded	2.2.12.03	**Gas Transport in Geosphere** Gas phase transport Gas phase release from Geosphere	1	N/A	1	**1**	0.73	0.73	0.73	0.73								
		2.2.14.00	**NUCLEAR CRITICALITY**																
51	Excluded	2.2.14.01	**Criticality in Far-Field** Formation of critical configuration	1	1	2	**1.38**	0	0	0	0								