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Generic Disposal System Modeling—Fiscal Year 2011 Progress Report

Fuel Cycle Research & Development

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

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Appendix E
FCT Document Cover Sheet

Name/Title of Deliverable/Milestone	*Generic Disposal System Modeling—Fiscal Year 2011 Progress Report* (report addresses two milestones) (1) Report describing the integrated generic disposal system environment (GDSE) model (SNL), M21UF034101 (2) General GoldSim model architecture report, M41UF035102
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This Deliverable was subjected to:

☒ Technical Review	☐ Peer Review
Technical Review (TR)	**Peer Review (PR)**
Review Documentation Provided	**Review Documentation Provided**
☐ Signed TR Report or,	☐ Signed PR Report or,
☐ Signed TR Concurrence Sheet or,	☐ Signed PR Concurrence Sheet or,
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Name and Signature of Reviewers

Peter Swift

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

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SUMMARY

The Used Fuel Disposition (UFD) Campaign supports the Fuel Cycle Technology (FCT) Program established by the United States Department of Energy Office of Nuclear Energy (DOE-NE). The mission of the UFD Campaign is to identify alternatives and conduct scientific research and technology development to enable storage, transportation and disposal of used nuclear fuel (UNF) and wastes generated by existing and future nuclear fuel cycles (DOE 2010c).

One element of the UFD Campaign is the generic disposal system modeling (GDSM) of different disposal environments and waste form options. GDSM has the following three-year goal (fiscal year (FY) 2014):

> *Have in place the necessary system architecture and computational environment to support the evaluation of postclosure risk. Maintain the flexibility in the system model architecture to meet the evolving needs of the DOE-NE/UFD mission. Provide risk information throughout the potential future phases of the mission including the following:*
>
> 1. *Viability*
> 2. *Screening*
> 3. *Selection*
> 4. *Characterization / Engineering Design*
> 5. *Licensing*

Currently, the GDSM team is investigating four main disposal environment options: mined repositories in three geologic media (salt, clay, and granite) and the deep borehole concept in crystalline rock (DOE 2010d). For each of these disposal options, the rock type is identified at a broad level. Salt includes both bedded and domal rocks; clay includes a broad range of fine-grained sedimentary rocks including shales, argillites, and claystones as well as soft clays; and granite includes a range of related crystalline rocks. The options for the waste stream being considered are UNF and high-level radioactive waste (HLW). Types of HLW include DOE high-level radioactive waste (DHLW) and commercial high-level radioactive waste (CHLW) generated from hypothetical reprocessing of commercial UNF.

The FY 2011 GDSM activities were conducted through two complementary work packages—*Generic Disposal System-Level Modeling* and *Repository Science/System-Level Analysis*—involving scientists from Sandia National Laboratories (SNL), Argonne National Laboratory (ANL), Los Alamos National Laboratory (LANL), and Lawrence Berkeley National Laboratory (LBNL).

The summary below describes the key GDSM accomplishments during FY 2011:

- Further developed the individual generic disposal system (GDS) models for salt, granite, clay, and deep borehole disposal environments. This work built on the generic disposal system environment (GDSE) modeling conducted in FYs 2009 and 2010. It was coordinated with the development of the initial Generic Performance Assessment Model (GPAM) architecture to facilitate the integration of the capabilities of the individual GDS models into the GPAM.
- Mapped the four individual GDS models in terms of the relevant UFD features, events, and processes
- Developed the initial GPAM architecture
  - Designed with the flexibility to evaluate different disposal environments as well as inventory/waste form options and to handle different levels of scientific detail and sophistication in a fashion that supports and utilizes evolving science efficiently
  - Created a Latin hypercube sampling (LHS) dynamic linked library (DLL) to work with the GPAM GoldSim® model file. The LHS DLL ensures reproducible results and allows the user more flexibility in selecting distributions to describe input data. The primary documentation for the LHS DLL is not this report, but another one entitled *Implementation of New Tools and*

Methods for Uncertainty Treatment (Sallaberry 2011). Sallaberry (2011) also documents the creation of a method for distinguishing between aleatory and epistemic uncertainty within GoldSim.

- Worked on the initial design for an external computational database called the GDS Parameter Database, which will be a key part of the long-term configuration management strategy. In the meantime, an interim strategy was established.

- Applied a systems engineering approach to learn from past PA efforts and to develop a more detailed description of the engineered barrier system (EBS) and systems architecture for consideration in the future
- Conducted process-level investigation of diffusion modeling in a clay repository. Data sets of parameters relevant to diffusive transport in clay were reviewed from literature and compiled. A review was completed of phenomenological approaches to model diffusive transport versus mechanistic approaches. An improved modeling approach was proposed to combine the advantages of both approaches.

This report presents these accomplishments and addresses two milestones:

- *Level 2 Milestone, Quality Rigor Level (QRL) 3*—Report describing the integrated generic disposal system environment (GDSE) model (SNL) (M21UF034101)
- *Level 4 Milestone, QRL3*—General GoldSim model architecture report (M41UF035102)

Results from the individual GDS models or GPAM are provided in this report solely to demonstrate the current capabilities of the models (e.g., what do they include, how do they function, what kinds of analyses can they do). These results should not be construed as being indicative of the true performance of a disposal system or compared to any regulatory performance objectives regarding repository performance. Drawing these types of conclusions is premature and not supported by the current pedigree of the models or the underlying data.

In fact, given the early development stage of the models, formal quality assurance (QA) processes are considered not applicable (N/A). In other words, the models are QA-N/A. Their development has not typically been subjected to the requirements of an established QA program from the FCT (DOE 2010b) or individual laboratories. However, the QA status will need to be reviewed if, as may happen in the future, there is a desire to use the software to support decision making within the UFD Campaign. Consideration will need to be given to ensuring the software is consistent with any UFD software QA requirements, which may include complying with the relevant laboratory software QA requirements, in force at the time.

With the development of the initial GPAM architecture, FY 2011 marks the start of the transition away from the four individual GDS models and to the holistic approach of GPAM. This transition will continue in FY 2012. Future refinements to the modeling capability for the different generic disposal environments are expected. However, once the transition to the GPAM is complete, those refinements or improvements will be made within the GPAM framework rather than the individual GDS models. FY 2012 plans also include further development of the functionality and structure of the GPAM system architecture, including a preliminary model interface to the GDS Parameter Database. Additionally, GDSM activities will utilize the current information available from the natural system, EBS, and loading management and design subject matter experts. Note that this early stage of model development has been done using GoldSim, but other framework tools are available as well. It is expected that a systematic evaluation will be conducted to investigate the capabilities of these other framework tools.

The GPAM is envisioned as being used to provide disposal risk information to DOE-NE/UFD decision makers to help support and defend decisions through the use of sensitivity and uncertainty studies and PA evaluations. Potential uses of GPAM include the following: (1) inform the prioritization of research and development activities within the UFD Campaign, (2) provide metric information regarding waste management that could be used by the FCT systems engineering effort in evaluating various advanced fuel cycle alternatives, and (3) provide viability assessments of Blue Ribbon Committee recommendations.

CONTENTS

FIGURES

TABLES

ACRONYMS

1D	one dimensional
2D	two dimensional
3D	three dimensional
ANL	Argonne National Laboratory
CHLW	commercial high-level radioactive waste
COx	Callovo-Oxfordian
DDL	diffuse double layer
DHLW	DOE high-level radioactive waste
DIR	diffusion of inert and reactive tracers
DLL	dynamic linked library
DOE	Department of Energy
EBS	engineered barrier system
EDZ	excavation disturbed zone
EPA	Environmental Protection Agency
ERB	Example Reference Biosphere
FCT	fuel cycle technology
FEHM	finite element heat and mass transfer
FEP	feature, event, and process
FY	fiscal year
GDS	generic disposal system
GDSE	generic disposal system environment
GDSM	generic disposal system modeling
GPAM	Generic Performance Assessment Model
HLW	high-level radioactive waste
HPC	high-performance computing
HTO	tritiated water
IAEA	International Atomic Energy Agency

ID	identification
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LHS	Latin hypercube sampling
LWR	light water reactor
MIC	microbially influenced corrosion
MS	Microsoft
MT	metric ton
MTHM	metric tons heavy metal
MTU	metric tons uranium
N/A	not applicable
NE	Office of Nuclear Energy
NEA	Nuclear Energy Agency
OPA	Opalinus Clay
PA	performance assessment
PAMINA	Performance Assessment Methodologies IN Application
PR	peer review
PWR	pressurized water reactor
QA	quality assurance
QRL	quality rigor level
R&D	research and development
RTD	residence time distribution
SCM	single-continuum model
SKB	Swedish Nuclear Fuel and Waste Management Company
SNF	spent nuclear fuel
SNL	Sandia National Laboratories
SCC	stress corrosion cracking
TBD	to be determined
THCMBR	thermal-hydrologic-chemical-mechanical-biological-radiological

TOc	Toarcian Clayey Formation
TR	technical review
TSPA	Total System Performance Assessment
UFD	used fuel disposition
UNF	used nuclear fuel
WIPP	Waste Isolation Pilot Plant

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USED FUEL DISPOSITION GENERIC DISPOSAL SYSTEM MODELING— FISCAL YEAR 2011 PROGRESS REPORT

1. INTRODUCTION

The generic disposal system modeling (GDSM) activities are focused on developing the capability of modeling different disposal environments and waste form options. The GDSM is part of the Used Fuel Disposition (UFD) Campaign, which itself is a part of the Fuel Cycle Technology (FCT) Program established by the United States Department of Energy Office of Nuclear Energy (DOE-NE).

The fiscal year (FY) 2011 GDSM activities involved scientists from Sandia National Laboratories (SNL), Argonne National Laboratory (ANL), Los Alamos National Laboratory (LANL), and Lawrence Berkeley National Laboratory (LBNL). The GDSM team built on the generic disposal system environment (GDSE) modeling conducted in FYs 2009 and 2010 (Wang and Lee 2010). The earlier work emphasized (1) development of four individual generic disposal system (GDS) performance assessment (PA) models for salt, granite, clay, and deep borehole disposal, and (2) detailed process-level studies to support generic PA model development, specifically in the clay environment. In FY 2011, the process-level studies were continued, with the subject being diffusion modeling in a clay repository. The work also included further development of the four individual GDS models. In addition, development began on an integrated model called the Generic Performance Assessment Model (GPAM). Ultimately, the goal is to migrate the capabilities of the individual GDS models to GPAM and then to move forward with development of GPAM, rather than the individual GDS models, as a resource for the UFD Campaign and the broader FCT Program.

This report documents the FY 2011 progress of GDSM activities with an emphasis on model development. These activities were conducted through the two complementary work packages, *Generic Disposal System-Level Modeling* and *Repository Science/System-Level Analysis*. This report addresses two milestones associated with these work packages:

- *Level 2 Milestone, Quality Rigor Level (QRL)3*—Report describing the integrated generic disposal system environment (GDSE) model (SNL) (M21UF034101)
- *Level 4 Milestone, QRL3*—General GoldSim model architecture report (M41UF035102)

The report is organized into six sections and two appendices:

- *Section 1*—Provides this introduction to the report.
- *Section 2*—Summarizes the effort to map the four individual GDS models in terms of relevant features, events, and processes (FEPs). The mapping was done using the UFD list of 208 FEPs identified in FY 2010 as being important to disposal system performance for various disposal alternatives (i.e., combinations of waste forms, disposal concepts, and geologic environments).
- *Section 3*—Documents the continued development of the four individual GDS models: 3.1 for the salt GDS model, 3.2 for the granite GDS model, 3.3 for the clay GDS model, and 3.4 for the deep borehole GDS model. These models are being developed with the flexibility to evaluate not only different properties, but also different waste streams/forms as well as different repository designs and engineered barrier configurations/materials that could be used to dispose of these wastes.
- *Section 4*—Describes the development of the GPAM architecture, including initial efforts regarding configuration management and the development of the GDS Parameter Database. The flexibility of

the individual GDS models is being incorporated into the GPAM, but with the added capability of eThisvaluating different disposal environments. The GPAM is also being designed with the flexibility to handle different levels of scientific detail and sophistication to meet the unique needs of future applications consistent with the goals of the UFD Campaign.

- *Section 5*—Provides a forward look at applying system engineering principles to the development of successively more detailed generic PA models (e.g., GPAM) in FY 2012 and beyond, with the specific example of the development of a more detailed engineered barrier system (EBS) architecture.
- *Section 6*—Presents the conclusions of the report including a brief summary of FY 2011 accomplishments and a look at future GDSM activities.
- *Appendix A*—Documents the progress on process-level modeling of diffusion in a clay repository. A review of the scientific literature for parameter data sets relevant to diffusive transport in clay was conducted, the result being a compilation of the data sets. In addition, a review was completed of phenomenological approaches to model diffusive transport versus mechanistic approaches. Results of this review are provided and a proposal made for an improved modeling approach that combines the advantages of both approaches.
- *Appendix B*—Provides the results to the FEPs mapping of the four individual GDS models. Table B-1 contains the results for the salt and granite GDS models, and Table B-2 contains the results for the clay and deep borehole GDS models.
- *Appendix C*—Documents preliminary estimates of the solubility and equilibrium linear sorption coefficient of some minor radionuclides for use in the disposal zone of the deep borehole GDS model. The estimates are also used for the salt GDS model as appropriate.

As mentioned above, the GDS models and GPAM are being developed with the capability of evaluating different waste form options. For clarity, this report uses the following terminology:

- *UNF*—Used nuclear fuel[a]
- *HLW*—High-level radioactive waste, which is the waste resulting from the reprocessing of UNF
- *DHLW*— DOE high-level radioactive waste
- *CHLW*—Commercial high-level radioactive waste (i.e., HLW generated by commercial reprocessing of UNF)

The FY 2011 GDSM activities included work (1) to develop a Latin Hypercube Sampling (LHS) dynamic linked library (DLL) for use with GoldSim® models and (2) to develop a method for distinguishing between aleatory and epistemic uncertainty within GoldSim. While the LHS DLL is mentioned in Section 4.2.2.3 of this report, the primary documentation for this work is a report entitled *Implementation of New Tools and Methods for Uncertainty Treatment* (Sallaberry 2011).

Results from the individual GDS models or GPAM are provided in this report solely to demonstrate the current capabilities of the models (e.g., what do they include, how do they function, what kinds of analyses can they do). These results should not be construed as being indicative of the true performance of a disposal system or compared to any regulatory performance objectives regarding repository performance. Drawing these types of conclusions is premature and not supported by the current pedigree of the models or the underlying data.

[a] In this report, UNF refers to fuel that has been withdrawn from a nuclear reactor following irradiation. After any potential interim storage period, the disposition of UNF may involve (1) providing constituent elements for reprocessing, and/or (2) permanent disposal in a geologic repository. UNF that is intended for permanent disposal may be referred to as spent nuclear fuel (SNF).

Given the early development stage of the models discussed in this report, formal quality assurance (QA) processes are not applicable (N/A). In other words, the models are considered QA-N/A. Their development has not typically been subjected to the requirements of an established QA program from the FCT (DOE 2010b) or individual laboratories. However, the QA status will need to be reviewed if, as may happen in the future, there is a desire to use the software to support decision making within the UFD Campaign. Consideration will need to be given to ensuring the software is consistent with any UFD software QA requirements, which may include complying with the relevant laboratory software QA requirements, in force at the time.

In addition, this early stage of model development has been done using GoldSim, but other framework tools are available as well. A systematic evaluation is planned for the future to investigate the capabilities of other potential framework tools.

2. FEPS MAPPING OF FOUR INDIVIDUAL GDS MODELS

The FEPs mapping activity consists of describing the four individual GDS models for salt, granite, clay, and deep borehole disposal (Section 3) in terms of the relevant FEPs. The goal is to provide the FEPs mapping as an aid to model developers in future GDSM efforts. The mapping also improves defensibility and confidence through increased transparency and traceability of the technical content. It provides a common framework to document the baseline capabilities of the four individual GDS models, which is important to help support the ongoing transition to the GPAM. Moreover, the mapping was completed using the UFD list of 208 FEPs identified in FY 2010 (Freeze et al. 2010) and updated in FY 2011 (Freeze et al. 2011a) as being important to disposal system performance for various disposal alternatives (i.e., combinations of waste forms, disposal concepts, and geologic environments). According to the UFD Campaign Research and Development (R&D) Roadmap (DOE 2010d, Section 1.2), these UFD FEPs provide the context for the identification of knowledge gaps, which can then be prioritized using system-level PA modeling:

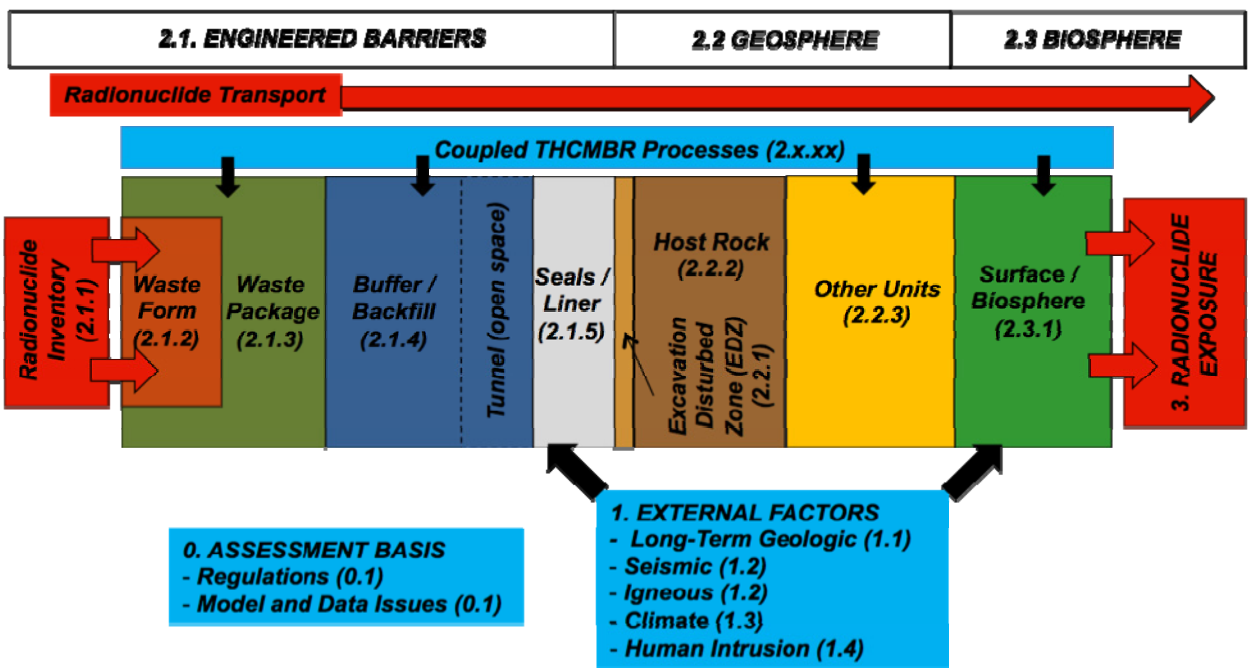
> *The current knowledge base can be mapped to corresponding FEPs to identify any gaps in knowledge. Potential information gaps, and hence research opportunities, lie in the areas of the data underlying, the representativeness of, confidence in, and defensibility of the mathematical representation of important phenomena in a safety assessment model used to support the safety case. An appropriate approach to identifying and prioritizing the importance of these information gaps is through system-level modeling which can then be used to evaluate the importance of these gaps with respect to overall disposal system performance. This results in a risk-informed prioritization of R&D needs where the results can be used to prioritize R&D projects towards the most critical knowledge gaps.*

Thus, using the UFD FEPs for mapping provides a common context recognized throughout the UFD Campaign and facilitates coordination between the GDSM team and other teams in support of the UFD mission.

The identification of these 208 UFD FEPs is documented in Freeze et al. (2010). The identification process involved the conceptualization of a system with components, domains, and phenomena common to most of the disposal alternatives considered. According to the FY 2010 progress report, “the phenomena that can affect the components and domains include, at a high level, the coupled THCMBR [thermal-hydrologic-chemical-mechanical-biological-radiological] processes that describe (1) waste form degradation and the source term, (2) radionuclide transport through the engineered components, (3) radionuclide transport through the geosphere, and (4) radionuclide transport, uptake, and health effects in the biosphere. In addition to their direct effects on radionuclide transport, the coupled THCMBR processes also influence the physical and chemical environments in the EBS, geosphere, and biosphere, which in turn affect water movement, degradation of EBS components, and radionuclide transport."

Each of the 208 UFD FEPs identified in the FY 2010 progress report is characterized by the following information (Freeze et al. 2010, Table A-1):

- *UFD FEP Number*—The numbering scheme is based on a hierarchical system that groups similar FEPs together. The numbers associated with various domains, features, events, and processes in Figure 2-1 correspond to the FEP numbering system. Across the disposal system domains there is a consistent structure and numbering scheme for the features (2.x.01 contains the first feature, 2.x.02 contains the second feature, etc.) and the processes (2.x.07 contains mechanical processes, 2.x.08 contains hydrologic processes, etc.).
- *Description*—The "Description" provides a coarse level of detail. The intent is that the "Description" be broad enough to be potentially applicable to the full range of disposal system alternatives. For example, "Sorption of Dissolved Radionuclides in the EBS" is potentially relevant to all waste form types and disposal concepts/geologic settings.
- *Associated Processes*—Each FEP is further defined by additional details under "Associated Processes". The level of detail collectively captured by the FEP Descriptions and Associated Processes is appropriate for the current FEP identification step of FEP analysis.



Source: Freeze et al. 2010, Figure 2.2.

Figure 2-1. Categorization of UFD FEPs

Until a licensing environment is reached, the FEPs information and level of detail will evolve as the UFD Campaign matures and develops, e.g., supporting viability, option screening, site selection, licensing and programmatic decisions. The current focus is on establishing FEPs at a level of detail necessary to support viability assessments.

The same information regarding each FEP was included in a Microsoft® (MS) Excel®-based tool developed to facilitate the mapping activity. However, the entries for a few FEPs were updated to maintain consistency with the FY 2011 UFD FEPs numbering and language (Freeze et al. 2011a). In addition, the naming terminology was changed slightly from UFD FEP Number, Description, and Associated Processes to UFD FEP ID, UFD FEP Title, and Process/Issue Description, respectively. For each of the four individual GDS models, the FEPs mapping tool provides three pick-list options for specifying whether a particular FEP is included: yes, partially, no. For mature models in a regulatory environment, a FEP is normally included or excluded. However, at this early stage of model development, the "partially" designation was added to better describe the situation in which only a portion of the capabilities needed to address a FEP have been implemented. There is also a "Description" field allowing for comment or explanation.

The results of the FEPs mapping activity are located in Appendix B. The FEPs mapping reflects the Freeze Point 2 versions of the individual GDS models and represents a step toward the level of detail needed to support viability assessments. As described in Section 4.2.3.2, the Freeze Point 2 versions of the models represent the farthest stage of development for FY 2011. If a particular FEP is included, the "Description" typically indicates where and how in the model the FEP is included. For partially included FEPs, the entry also indicates what aspects of the FEP are included. For FEPs (or aspects of FEPS) that are not included, the entry may provide additional information such as whether there are plans to include the FEP in the future or whether such inclusion is unlikely. It is important to remember that the capabilities of the individual GDS models are being integrated into the GPAM. Afterwards, improvements to the capability to simulate a particular disposal option, including the inclusion of new FEPs, will be done in GPAM. Therefore, any discussion in the results tables about potentially including a FEP in an individual model should be viewed in the context of adding the FEP to the modeling capability for that disposal option rather than to that specific model, since implementation will actually be in the GPAM.

Unlike the four individual models, the GPAM was not selected for FEPs mapping at this time because of its early stage of development. Moreover, the transition to the GPAM involves incorporating the capability to model all of the FEPs included in the individual GDS models. Consideration can be given to mapping GPAM in the future when it is more stable and the effort more likely to yield useful results. In the meantime, there is a crosswalk showing how aspects of the four individual models are being integrated into GPAM (Table 4-5).

Note that there have been no FEP screening evaluations conducted as yet. Currently, FEP evaluations are limited to an ongoing effort to compile existing information that might be relevant in identifying important considerations (i.e., phenomena) for the range of potential disposal system designs (Freeze et al. 2010, Section 3). Because there have been no formal screening evaluations, the decision to include or exclude a FEP or aspects of a FEP at this point is based solely on the expert opinions of subject matter experts. The current emphasis is on building a PA capability. Screening evaluations can be conducted at some point in the future as the modeling effort evolves to meet the needs of the UFD Campaign and as relevant regulations are identified.

3. FOUR INDIVIDUAL GDS MODELS

The GDSM effort is focused on developing the tools needed to conduct and analyze comparative studies of different disposal environments and waste forms options. The modeling activities summarized in this section are focused on four generic disposal environments, i.e. clay, granite, salt, and deep borehole. For each of these disposal options, the rock type is identified at a broad level. Salt includes both bedded and domal rocks; clay includes a broad range of fine-grained sedimentary rocks including shales, argillites, and claystones as well as soft clays; and granite includes a range of related crystalline rocks. The immediate goal of the generic repository studies is to develop modeling tools to evaluate the viability of different options and to improve understanding of potential repository system response to processes relevant to the long-term disposal of UNF and HLW.

There are multiple uses for building the capability to model these generic disposal environments within the UFD Campaign:

- Inform the prioritization of R&D activities
- Provide the basis for system level PA of varied disposal environments
- Provide risk and other metric information for assessing potential performance of different disposal environments being evaluated by the UFD Campaign

To support these uses, the GDS models and associated database are being developed with the flexibility to evaluate different host rock properties, different waste streams/forms, and different repository designs and engineered barrier configurations/ materials that could be used to dispose of the wastes. This section describes the status of the individual GDS models, at their current stage of development. Each subsection includes a description of the conceptual model of the disposal environment and the mathematical implementation of that conceptual model. The models draw on data available from the published literature to the extent possible. Existing scientific models describing the various repository processes and the parameter values supporting them will be replaced as appropriate and as data become available from other UFD work packages (e.g., Natural Systems and EBS).

Each main subsection includes preliminary results and discussion of results for the models as a demonstration of capability. There is also a discussion of confidence-building activities that have been conducted. If available, published results from the literature are used for comparison in these confidence-building activities. Some sensitivity analyses have also been performed to improve the understanding of the models. At this stage, it is important that model results not be construed as being indicative of the true performance of a disposal system or compared to any regulatory performance objectives regarding repository performance. Drawing these types of conclusions is premature and not supported by the current pedigree of the models or the underlying data.

In the future these models will be incorporated into GPAM, which is described in Section 4. The individual GDS models will be retired, and all calculations and further model development will be completed using GPAM.

3.1 Salt GDS Model

The development of the salt GDS model, the model implementation, and the model analysis results are discussed in the subsections of Section 3.1.

3.1.1 Introduction

The immediate goal of the generic salt repository study is to develop the necessary modeling tools to evaluate and improve understanding on the repository system response and processes relevant to long-term disposal of UNF and HLW in salt. This initial phase of study considered, where applicable, representative geologic settings and features adopted from literature data for salt repository sites. The conceptual model and scenario for radionuclide release and transport from a salt repository was developed utilizing literature data. The current version of the salt GDS model consists of four major model components: source term, near field, far field, and biosphere. The salt generic repository model was implemented in GoldSim (GoldSim Technology Group 2009). The repository performance analysis was performed probabilistically, with 100 realizations for each case and for a time period of 1,000,000 yr.

The model analysis discussion includes the key attributes of a salt repository that are potentially important to the long-term safe disposal of UNF and HLW. It also discusses the model analysis results showing the repository response to the effects of different waste stream types (commercial UNF, DHLW, and CHLW), and two different radionuclide release scenarios (nominal (or undisturbed) and human intrusion (or disturbed)). In addition, there is a discussion of the identified knowledge gaps and paths forward for future R&D efforts to advance understanding of salt repository system performance for UNF and HLW disposal. Section 3.1.2 describes the salt conceptual model for each of the model components and scenarios considered. Section 3.1.3 describes the implementation of the conceptual models. Section 3.1.4 demonstrates the use of the model, and Section 3.1.5 provides a summary and conclusions relevant to the salt GDS model. The capabilities of the salt GDS model are being incorporated into the GPAM (Section 4) along with the capabilities of the models for the granite, clay, and deep borehole repository options. Afterwards, GPAM can be used to provide guidance on the development of strategy for long-term disposal of UNF and HLW in a salt repository.

3.1.2 Model Description

3.1.2.1 Conceptual Model

Because comprehensive information is readily available for the Waste Isolation Pilot Plant (WIPP), the geologic settings and features of the generic salt repository were adopted, where applicable, from the WIPP site (Helton et al. 1998). Figure 3.1-1 shows a schematic of the geologic setting and the conceptual model for radionuclide release and transport in a generic salt repository. The model assumes that repository is located in a bedded salt formation in a saturated, chemically reducing environment. The waste package is placed horizontally in an emplacement alcove and backfilled with crushed salt. Over a period of time following the emplacement, the confined space around the waste disposal area will be slowly closed by creep deformation of salt rock, and the crushed salt backfill will undergo consolidation. This would result in close contact of the waste package with the consolidated salt rock and potential encapsulation of the waste package by salt rock.

A horizontal interbed with a significant thickness of relatively more permeable anhydrite is assumed to exist below the repository, and runs in parallel with the repository horizon to an extended distance; a carbonate aquifer is assumed to exist above the repository. Two scenarios are considered for repository radionuclide release and transport: the reference (or nominal) case, and the disturbed case. The reference case releases radionuclides by a sequence of typical processes that are expected to occur in a generic salt repository; the case assumes that the interbed provides the major pathway for radionuclide release and transport from the repository, and this is supported by the model results from WIPP (Helton et al. 1998). The disturbed case considers a process that results in a fast pathway for radionuclides to the far field, and the case is represented by a “stylized” human intrusion scenario, which assumes that a single borehole penetrates a waste package and a pressurized brine reservoir below the repository and dissolved radionuclides are released directly into the overlying aquifer. The current human intrusion scenario does not consider the potential dose impacts of the waste that could be brought up directly to the surface as a result of the drilling activities. The modeling assumption for the disturbed case will be updated as the study progresses.

In the postclosure repository, the waste decay heat would cause near-field brines (present in small quantities in undisturbed bedded salt as pore water) to boil during the peak thermal perturbation period, driving the water away from the waste disposal area leaving behind salt minerals in the pore space. This would create a dry-out zone around the waste disposal area, and its duration would depend mostly on the waste heat output characteristics, repository thermal loading, and thermal characteristics of the salt. The thermal perturbation and its associated moisture movement would also enhance creep deformation of salt and closure of the open space of the waste disposal area. As the temperatures decrease following the peak, brines could start flowing toward and into the waste disposal area driven by higher (i.e., near lithostatic) pore pressure in the far field.

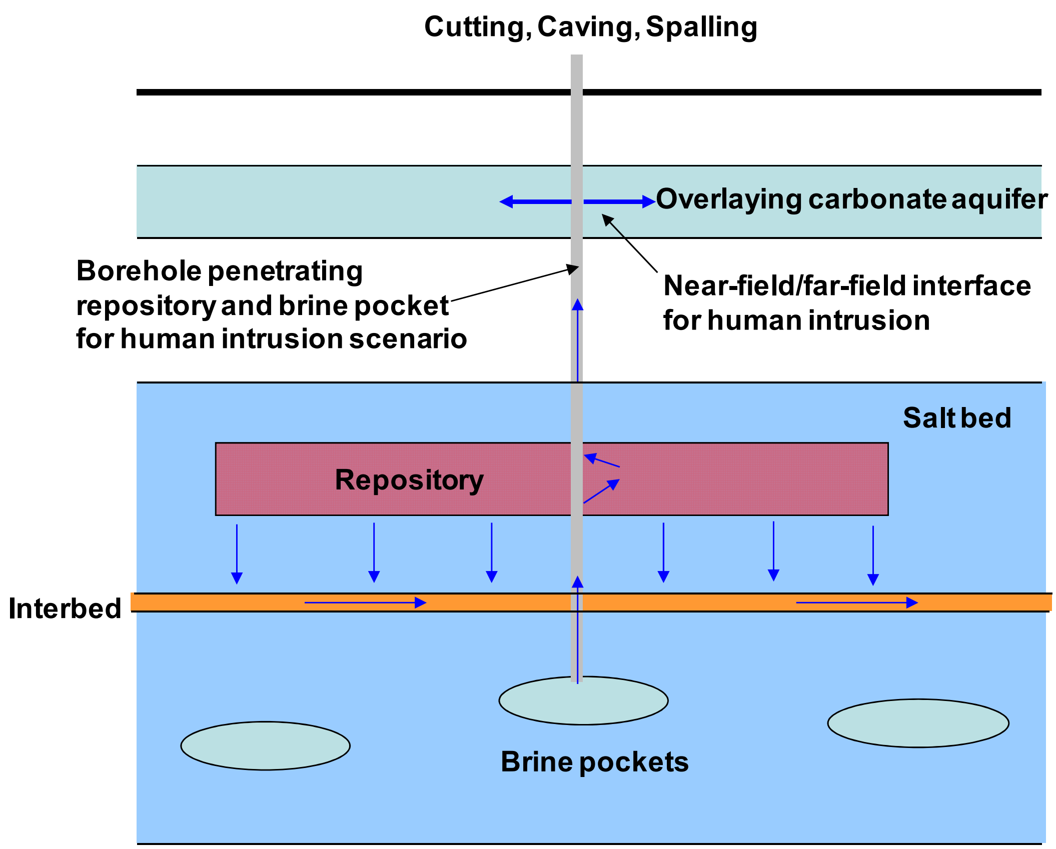


Figure 3.1-1. A Schematic Showing the Conceptual Model for Radionuclide Release and Transport from a Salt Generic Repository

Corrosion of waste package and other engineered materials in the disposal area could be enhanced when in contact with concentrated brines at elevated temperatures, and gases will be generated as a result of the corrosion under chemically reducing conditions. Subsequent to waste package corrosion failure, corrosion of the waste form, its canister, and waste package internal structure materials would occur, releasing radionuclides and generating additional corrosion gases. Combined actions of the corrosion gas generation and decreasing confined space in the disposal area by salt creep deformation would pressurize the disposal area; this could result in brine flows and potential transport of dissolved radionuclides away from the disposal areas to some distance.

Because information on thermal perturbation and the associated repository processes such as brine flow, salt creeps, corrosion, gas generation, etc. for a representative generic salt repository are not available, the model assumes an isothermal condition at 25°C for the generic repository. Because of the lack of information at this early stage, the current salt GDS model does not consider conservatively the barrier performance of the waste package and waste form canisters. They are assumed to fail immediately (at time zero), and waste form degradation occurs from the beginning of the analysis. Results from these analyses are only meant for demonstration purposes and should not be used to support any decisions. The performance of these barriers will be included in future GDSM efforts as information becomes available from subject matter experts involved in other UFD work packages.

3.1.2.2 Waste Inventory

Three different types of UNF and HLW are considered in the source-term model: commercial UNF, existing DHLW, and "hypothetical" CHLW of commercial UNF. The source-term model radionuclide inventory analysis is based on the detailed fuel cycle waste inventory analysis provided by Carter and Luptak (2010). The salt GDS source-term model inventory includes 36 radionuclides, accounting for both in-growth of daughters and isotopic mixing among radionuclides.

Commercial UNF Inventory—The once-through fuel cycle waste inventory analysis considers four scenarios to evaluate the projected increases in the commercial light water reactor (LWR) UNF inventory. The four once-through fuel cycle scenarios are considered to provide a wide range of LWR fuel inventory for use in future analysis (Carter and Luptak 2010, Section 3.2). The salt GDS source-term inventory analysis is based on once-through fuel cycle inventory Scenario 1, which assumes no replacement of existing nuclear generation reactors. Selection of this UNF inventory scenario for the salt GDS source-term inventory analysis is arbitrary, and it can be revised as needed in future analyses. For this scenario, a total of 140,000 metric tons uranium (MTU) used fuel is estimated to be discharged from reactors (Carter and Luptak 2010, Table 3-5). Out of the total inventory, 91,000 MTU is from the pressurized water reactors (PWRs) UNF with an estimated total of 209,000 assemblies. This is equivalent to 0.435 MTU per PWR assembly.

For simplification of the source-term model, the total inventory was converted to an equivalent PWR inventory, resulting in a total of 321,540 PWR assemblies. The source-term model assumes that a waste package contains 10 PWR assemblies; therefore a total of 32,154 waste packages are needed for disposal of the commercial UNF (140,000 MTU).

The isotopic inventory of the UNF is assumed to be represented by the PWR fuel with a burn-up of 60 GWd/MTHM (metric tons heavy metal) and 4.73% enrichment and aged 30 yr after discharge from reactor (Carter and Luptak 2010, Table C-1). The isotopic inventory for the radionuclides of the commercial UNF included in the source-term model is shown in Table 3.1-1.

Table 3.1-1. Isotopic Inventory for Commercial UNF for Salt GDS Source-Term Model

Isotope	Half Life (yr)	Fractional Mass Inventory	Isotope Mass per Waste Package (g)
^{227}Ac	2.18E+01	2.7469E-13	1.1960E-06
^{241}Am	4.32E+02	8.7003E-04	3.7882E+03
^{243}Am	7.37E+03	1.8796E-04	8.1841E+02
^{14}C	5.71E+03	3.1524E-07	1.3726E+00
^{36}Cl	3.01E+05	3.4808E-07	1.5156E+00
^{245}Cm	8.50E+03	6.6221E-06	2.8833E+01
^{135}Cs	2.30E+06	5.3570E-04	2.3325E+03
^{137}Cs	3.01E+01	7.2561E-04	3.1593E+03
^{129}I	1.70E+07	2.1754E-04	9.4720E+02
^{93}Nb	1.36E+01	4.9591E-04	2.1592E+03
^{237}Np	2.14E+06	8.5892E-04	3.7398E+03
^{231}Pa	3.25E+04	7.1103E-10	3.0959E-03
^{210}Pb	2.26E+01	7.8324E-15	3.4103E-08
^{107}Pd	6.50E+06	2.8663E-04	1.2480E+03
^{238}Pu	8.77E+01	3.4170E-04	1.4878E+03
^{239}Pu	2.41E+04	5.1487E-03	2.2418E+04
^{240}Pu	6.54E+03	2.8427E-03	1.2377E+04
^{241}Pu	1.44E+01	2.6198E-04	1.1407E+03
^{242}Pu	3.76E+05	5.6750E-04	2.4709E+03
^{226}Ra	1.60E+03	2.2081E-12	9.6141E-06
^{228}Ra	6.70E+00	1.4339E-18	6.2431E-12
^{126}Sb	3.61E-05	1.6470E-12	7.1713E-06
^{79}Se	6.50E+04	7.2769E-06	3.1684E+01
^{126}Sn	1.00E+05	3.4663E-05	1.5092E+02
^{90}Sr	2.91E+01	3.0809E-04	1.3414E+03
^{99}Tc	2.13E+05	8.8739E-04	3.8638E+03
^{229}Th	7.90E+03	4.4252E-12	1.9267E-05
^{230}Th	7.54E+03	1.5838E-08	6.8961E-02
^{232}Th	1.41E+10	4.2412E-09	1.8466E-02

Table 3.1-1. Isotopic Inventory for Commercial UNF for Salt GDS Source-Term Model (continued)

Isotope	Half Life (yr)	Fractional Mass Inventory	Isotope Mass per Waste Package (g)
^{232}U	6.89E+01	3.1642E-09	1.3777E-02
^{233}U	1.59E+05	9.7002E-09	4.2235E-02
^{234}U	2.45E+05	2.1220E-04	9.2392E+02
^{235}U	7.04E+08	3.7329E-03	1.6253E+04
^{236}U	2.34E+07	4.3349E-03	1.8874E+04
^{238}U	4.46E+09	6.3215E-01	2.7524E+06
^{93}Zr	1.53E+06	1.0193E-03	4.4382E+03

DHLW Inventory—All existing DHLW is assumed to be immobilized in borosilicate glass logs as it is the candidate waste form (Carter and Luptak 2010). The source-term model uses the best-estimate projected total number of DHLW canisters documented in the fuel cycle inventory analysis report (Carter and Luptak 2010, Table 2-2); the best estimate projection is 25,016 canisters. The source-term model assumes that each waste package contains 5 DHLW canisters; therefore a total of 5,003 waste packages are needed for disposal of the DHLW.

The isotope inventory of the DHLW is given for each radionuclide in terms of the total radioactivity (*Ci*) in the fuel cycle inventory analysis report (Carter and Luptak 2010, Table F-1). The radioactivity was converted to the equivalent mass (m_i) for each radionuclide as follows:

$$m_i\,(g) = \frac{A_i \cdot t_{\frac{1}{2},i} \cdot MW_i}{0.693 \cdot N_A} \qquad \text{Eq. 3.1-1}$$

where A_i is the radioactivity of radionuclide *i*, $t_{1/2,i}$ is the half-life of radionuclide *i*, MW_i is the molecular weight of radionuclide *i*, and N_A is the Avogadro constant (6.023×10^{23}). The total mass of radionuclides of the existing DHLW is estimated 1,759 metric tons (MT). This gives 0.07 MT of radionuclides per DHLW canister, and 0.35 MT of radionuclides per waste package. The isotopic inventory per DHLW canister and per waste package is given in Table 3.1-2. The fuel cycle inventory analysis reports zero inventory for ^{36}Cl for the DHLW (Carter and Luptak 2010), and the inventory analysis is currently under review to confirm the ^{36}Cl inventory.

Table 3.1-2. Isotopic Inventory for DHLW for Salt GDS Source-Term Model

Isotope	Half Life (yr)	Fractional Mass Inventory	Isotope Mass per Canister (g)	Isotope Mass per Waste Package (g)
^{227}Ac	2.18E+01	1.139E-09	8.010E-05	4.005E-04
^{241}Am	4.32E+02	4.022E-04	2.829E+01	1.414E+02
^{243}Am	7.37E+03	2.732E-05	1.922E+00	9.608E+00
^{14}C	5.71E+03	1.747E-08	1.228E-03	6.142E-03
^{36}Cl	3.01E+05	0.000E+00	0.000E+00	0.000E+00
^{245}Cm	8.50E+03	5.428E-07	3.817E-02	1.909E-01
^{135}Cs	2.30E+06	1.759E-03	1.237E+02	6.184E+02
^{137}Cs	3.01E+01	2.219E-03	1.561E+02	7.804E+02
^{129}I	1.70E+07	1.802E-04	1.268E+01	6.338E+01
^{93}Nb	1.36E+01	0.000E+00	0.000E+00	0.000E+00
^{237}Np	2.14E+06	3.004E-04	2.113E+01	1.056E+02
^{231}Pa	3.25E+04	3.452E-06	2.427E-01	1.214E+00
^{210}Pb	2.26E+01	1.317E-13	9.264E-09	4.632E-08
^{107}Pd	6.50E+06	2.188E-05	1.539E+00	7.696E+00
^{238}Pu	8.77E+01	2.070E-04	1.456E+01	7.279E+01
^{239}Pu	2.41E+04	1.749E-03	1.230E+02	6.151E+02
^{240}Pu	6.54E+03	1.865E-04	1.312E+01	6.559E+01
^{241}Pu	1.44E+01	2.468E-06	1.736E-01	8.678E-01
^{242}Pu	3.76E+05	2.154E-05	1.515E+00	7.573E+00
^{226}Ra	1.60E+03	5.747E-11	4.042E-06	2.021E-05
^{228}Ra	6.70E+00	4.563E-11	3.209E-06	1.604E-05
^{126}Sb	3.61E-05	5.728E-12	4.029E-07	2.014E-06
^{79}Se	6.50E+04	3.085E-04	2.169E+01	1.085E+02
^{126}Sn	1.00E+05	1.215E-04	8.548E+00	4.274E+01
^{90}Sr	2.91E+01	9.262E-04	6.514E+01	3.257E+02
^{99}Tc	2.13E+05	3.212E-03	2.259E+02	1.129E+03
^{229}Th	7.90E+03	9.980E-09	7.019E-04	3.509E-03
^{230}Th	7.54E+03	4.546E-09	3.197E-04	1.599E-03
^{232}Th	1.41E+10	9.894E-02	6.958E+03	3.479E+04

Table 3.1-2. Isotopic Inventory for DHLW for Salt GDS Source-Term Model (continued)

Isotope	Half Life (yr)	Fractional Mass Inventory	Isotope Mass per Canister (g)	Isotope Mass per Waste Package (g)
^{232}U	6.89E+01	1.141E-09	8.022E-05	4.011E-04
^{233}U	1.59E+05	5.300E-05	3.727E+00	1.864E+01
^{234}U	2.45E+05	7.431E-05	5.226E+00	2.613E+01
^{235}U	7.04E+08	3.732E-03	2.625E+02	1.312E+03
^{236}U	2.34E+07	2.863E-04	2.014E+01	1.007E+02
^{238}U	4.46E+09	8.821E-01	6.204E+04	3.102E+05
^{93}Zr	1.53E+06	1.739E-03	1.223E+02	6.115E+02

CHLW Inventory—The fuel cycle inventory analysis report discusses several candidate reprocessing methods for commercial UNF and their potential waste streams (Carter and Luptak 2010, Section 4). For simplification, the following assumptions or steps were made to calculate the isotopic inventory of CHLW resulting from "hypothetical" reprocessing of commercial UNF in this report:

- Ninety nine percent (99%) of uranium and plutonium are recovered. All others including minor transuranic elements and fission products of the commercial UNF inventory (140,000 MTU) remain in the waste streams.
- The fractional isotopic mass inventory of the CHLW is calculated after removing 99% of the uranium and plutonium mass from the commercial UNF inventory. As in the DHLW, no inventory is assumed for ^{36}Cl.
- CHLW is immobilized in borosilicate glass, the same as for the DHLW.
- CHLW is encapsulated at the same radionuclide mass loading as for the DHLW (i.e., 0.07 MT radionuclide mass per canister).

Note that the above assumptions result in higher concentrations of fission products in the CHLW waste streams and glass waste form than the DHLW. The total radionuclide mass of the CHLW is estimated 1,426 MT (after removing 99% of uranium and plutonium). With a radionuclide mass loading of 0.07 MT per canister, this is equivalent to a total of 20,276 canisters. The source-term model assumes that each waste package contains five CHLW canisters; therefore a total of 4,055 waste packages are needed for disposal. The isotopic inventory for CHLW is given in Table 3.1-3.

Table 3.1-3. Isotope Inventory for CHLW for Salt GDS Source-Term Model

Isotope	Half Life (yr)	Fractional Mass Inventory	Isotope Mass per Canister (g)	Isotope Mass per Waste Package (g)
^{227}Ac	2.18E+01	2.6969E-11	1.8967E-06	9.4833E-06
^{241}Am	4.32E+02	8.5419E-02	6.0073E+03	3.0037E+04
^{243}Am	7.37E+03	1.8454E-02	1.2978E+03	6.4892E+03
^{14}C	5.71E+03	3.0950E-05	2.1766E+00	1.0883E+01
^{36}Cl	3.01E+05	0.0000E+00	0.0000E+00	0.0000E+00
^{245}Cm	8.50E+03	6.5015E-04	4.5724E+01	2.2862E+02
^{135}Cs	2.30E+06	5.2594E-02	3.6989E+03	1.8494E+04
^{137}Cs	3.01E+01	7.1239E-02	5.0101E+03	2.5051E+04
^{129}I	1.70E+07	2.1358E-02	1.5021E+03	7.5104E+03
^{93}Nb	1.36E+01	6.8717E-07	4.8327E-02	2.4164E-01
^{237}Np	2.14E+06	8.4328E-02	5.9306E+03	2.9653E+04
^{231}Pa	3.25E+04	6.9808E-08	4.9094E-03	2.4547E-02
^{210}Pb	2.26E+01	7.6897E-13	5.4080E-08	2.7040E-07
^{107}Pd	6.50E+06	2.8141E-02	1.9791E+03	9.8956E+03
^{238}Pu	8.77E+01	3.3547E-05	2.3593E+00	1.1797E+01
^{239}Pu	2.41E+04	5.0549E-04	3.5550E+01	1.7775E+02
^{240}Pu	6.54E+03	2.7909E-04	1.9628E+01	9.8141E+01
^{241}Pu	1.44E+01	2.5721E-05	1.8089E+00	9.0446E+00
^{242}Pu	3.76E+05	5.5717E-05	3.9184E+00	1.9592E+01
^{226}Ra	1.60E+03	2.1679E-10	1.5246E-05	7.6230E-05
^{228}Ra	6.70E+00	1.4077E-16	9.9004E-12	4.9502E-11
^{126}Sb	3.61E-05	1.6170E-10	1.1372E-05	5.6861E-05
^{79}Se	6.50E+04	7.1444E-04	5.0245E+01	2.5122E+02
^{126}Sn	1.00E+05	3.4031E-03	2.3933E+02	1.1967E+03
^{90}Sr	2.91E+01	3.0248E-02	2.1273E+03	1.0636E+04
^{99}Tc	2.13E+05	8.7123E-02	6.1272E+03	3.0636E+04
^{229}Th	7.90E+03	4.3446E-10	3.0554E-05	1.5277E-04
^{230}Th	7.54E+03	1.5550E-06	1.0936E-01	5.4680E-01
^{232}Th	1.41E+10	4.1639E-07	2.9284E-02	1.4642E-01

Table 3.1-3. Isotope Inventory for CHLW for Salt GDS Source-Term Model (continued)

Isotope	Half Life (yr)	Fractional Mass Inventory	Isotope Mass per Canister (g)	Isotope Mass per Waste Package (g)
^{232}U	6.89E+01	3.1066E-10	2.1848E-05	1.0924E-04
^{233}U	1.59E+05	9.5236E-10	6.6977E-05	3.3489E-04
^{234}U	2.45E+05	2.0833E-05	1.4652E+00	7.3258E+00
^{235}U	7.04E+08	3.6649E-04	2.5775E+01	1.2887E+02
^{236}U	2.34E+07	4.2559E-04	2.9931E+01	1.4966E+02
^{238}U	4.46E+09	6.2063E-02	4.3648E+03	2.1824E+04
^{93}Zr	1.53E+06	1.0008E-01	7.0381E+03	3.5191E+04

3.1.2.3 Waste Package Configuration

The waste package configuration for the salt GDS source-term model is based on the waste cask design for SNF of the German salt disposal program (Janberg and Spilker 1998). The outer diameter of a waste package is 1.56 m, and the outer length is 5.5 m. Each waste package is assumed to hold 10 PWR UNF assemblies, 5 DHLW canisters, or 5 CHLW canisters. As noted in Section 3.1.2.1, the current salt GDS analysis does not consider the barrier performance of the waste package. The assumed waste package configuration is used in other submodel components such as repository footprint and waste package radionuclide inventory.

3.1.2.4 Reference Repository Layout

For simplification, it is assumed that the repository has a square footprint. Knowing the total number of waste packages (N_{WP}) to be disposed of in the repository, the side length (L_{Rep}) of a square repository footprint can be calculated as follows:

$$\frac{L_{Rep}}{L_{WP}+S_{WP}} \times \frac{L_{Rep}}{S_{drift}} = N_{WP} \qquad \text{Eq. 3.1-2}$$

where L_{WP} is the length of waste package (5.5 m), S_{WP} is the spacing between waste packages (6 m), and S_{drift} is the spacing between emplacement tunnels (25 m). The waste package length is specified in Section 3.1.2.3. The values for the waste package spacing and emplacement tunnel spacing were taken from the Swedish Nuclear Fuel and Waste Management Company (SKB) repository design (Claesson and Probert 1996; SKB 2006).

3.1.2.5 Waste Form Degradation

The three different waste inventories described in Section 3.1.2.2 contain two different waste form types. For commercial UNF, the waste form is the UNF matrix, which is predominantly UO_2. For the DHLW and CHLW, the waste form is borosilicate glass. For both waste form types, the waste form degradation in the source-term model is represented with an annual fractional degradation rate (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates that could be expected in a generic salt repository environment. The generic salt repository is expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. In the current salt GDS model, for a given realization, a (sampled) constant degradation rate is applied to the entire inventory; no temperature or spatial dependence is modeled at this time.

For the commercial UNF waste form, uncertainty in the degradation rate is modeled with a log-triangular distribution with the mode of $10^{-7}\ yr^{-1}$ and lower and upper bounds of $10^{-8}\ yr^{-1}$ and $10^{-6}\ yr^{-1}$ respectively. The rate range is from the SKB SNF degradation model for its repository situated in a chemically reducing environment (SKB 2006, Sections 10.5.3 and 10.6.4).

For the borosilicate glass waste form, degradation is much less sensitive to the redox condition of water contacting the waste form. A fractional degradation rate model was developed using the literature data for degradation of similar glasses exposed in geologic environments (Ojovan et al. 2005; BSC 2004, Table 6-14). The rate model is expressed as log-uniform distribution with the minimum and maximum values of $3.4 \times 10^{-6}\ yr^{-1}$ and $3.4 \times 10^{-3}\ yr^{-1}$ respectively.

Waste form degradation is assumed to release radionuclides into a large uniformly mixed container representative of the source-term water volume. The source-term water volume is obtained by multiplying the source-term bulk volume by its porosity. The dissolved concentrations of radionuclides in the source term mixing cell are then calculated based on the mass of radionuclides released from the waste form, the source-term water volume, and the radionuclide solubility. In the salt GDS source-term model, the source-term mixing cell is conceptualized to include the bulk volume of all of the near-field components (waste form, waste package, crushed salt backfill, near-field salt rock, etc.). This is a reasonable assumption for the current GDS analysis, considering that waste package performance is not taken into account for the analysis and that the entire waste inventory becomes available for reactions in the near field from time zero. As the model matures and information becomes available, more realistic representations of the processes will replace this initial simplified approach.

3.1.2.6 Near Field

As described in Section 3.1.2.5, the source-term bulk volume in the salt GDS model is represented by the near-field bulk volume. The near-field bulk volume is defined as the square repository footprint area (Section 3.1.2.4) times the near-field height. For a salt GDS, in which the remaining space of the waste emplacement area is likely closed by the salt creep deformation, the near-field height is defined as the waste package outer diameter. The near-field height currently used in the salt GDS source-term model is arbitrary and will be updated as needed in future analyses. The disturbed rock zone that will develop around the excavation (i.e., the excavation disturbed zone (EDZ)) is not included in the near-field model as the zone will be healed by salt consolidation processes. The so-defined near field has two major constituents: (1) degraded engineered materials (e.g., waste form, waste package, crushed salt backfill, etc.), and (2) host rock. The salt GDS source-term model calculates the water volume available in each of the two constituents by multiplying the bulk volume of each constituent with its respective porosity. The total water volume available in the near field is the sum of the water volume in each constituent.

The near-field brine will experience elevated temperature conditions from the thermal perturbations caused by the decay heat of emplaced waste. A study was conducted for the conduction-only thermal analysis of a generic salt repository for disposal of vitrified HLW from reprocessing of commercial UNF (Clayton and Gable 2009). However, the analysis was performed only for the first 50-yr period after waste emplacement, and it does not provide long-term (repository time-scale) thermal-hydrologic conditions necessary for the salt GDS analysis. Because the near-field thermal evolution information is not available, the salt GDS analysis assumes the site ambient temperature of 25°C for the near-field exposure condition.

The current salt GDS model assumes conservatively no radionuclide sorption on the near-field constituent materials. As many radionuclides are known to sorb on geologic materials and, in particular, strongly on metal corrosion products in chemically reducing condition, the impact of this conservative assumption needs to be evaluated in a future iteration of the salt GDS performance analysis.

Dissolved radionuclide concentrations in the near field are determined by the mass of radionuclides released from the waste form (constrained by the waste form degradation rate), the volume of brine available in the near field, and the radionuclide solubility if it is subject to its solubility limit. Radionuclide solubility is affected at varying degrees by various geochemical conditions, including redox condition of contacting water, temperature, pH, and presence and concentration of other dissolved species. As an initial effort to address the effect of geochemical conditions on radionuclide solubility, the salt GDS analysis considers two redox conditions for salt brine: (1) chemically reducing condition brine, and (2) less reducing or slightly oxidizing brine. Solubility calculations for these two redox conditions were based on the chemical compositions of two well-studied brines from the WIPP site: (1) a concentrated brine derived either from the repository horizon or the pressurized brine reservoir beneath the repository, representative of a chemically reducing condition; and (2) a dilute brine from the interface between the near field and the far field, representative of a much less reducing condition. The chemical compositions of the two brines are given in Wang and Lee (2010). Solubility calculations for U, Pu, Am, Np, Th, and Sn were performed with computer code EQ3/6 and an enhanced Pitzer thermodynamic database (Wolery and Jarek 2003). Details of the solubility analysis for the representative groundwaters are found elsewhere (Wang and Lee 2010). In the salt GDS model, the reducing condition is representative of the brine in the near field, and the less reducing or slightly oxidizing condition is representative of the brine away from the near field (i.e., in the interface area between the near field and far field, in the far-field interbed, and in the overlying aquifer).

The resulting elemental solubilities for the ambient temperature condition of 25°C applied to the salt GDS near-field model are shown in Table 3.1-4. In addition to the calculated solubilities for the elements described above, elemental solubilities for other radionuclides (Ac, C, Cl, Cm, Cs, I, Nb, Pa, Pd, Ra, Sb, Se, Sr, and Zr) are shown. Elements C, Ra and Sr are implemented as unlimited solubility in the near-field model because their solubility calculations have not been completed. Elemental solubilities corresponding to the salt GDS interface area, far-field interbed and overlying aquifer are shown later in Table 3.1-6. The impact of the ambient-temperature condition assumption and the use of the 25°C solubility for the salt GDS near-field model will be evaluated when the necessary information becomes available.

The salt GDS model includes a region of interface rock block between the repository and underlying interbed (Figure 3.1-1). The interface rock region is assumed to have the same area as the repository footprint and a thickness of 5 m. The salt GDS model simulates release of dissolved radionuclides from the repository near field to the interface region and subsequent transport through the interface region, both by diffusion and advection. As for the near field, the model conservatively assumes no sorption of radionuclides in the interface region, and the far-field elemental solubility (Section 3.1.2.7) is applied to radionuclides in the interface region.

The brine flow rates in the near-field and interface region are sampled from 100 time-dependent brine flow rate histories, which are abstracted from detailed brine migration process simulations as discussed in Section 3.1.3. The salt GDS model parameters for the near-field and interface region are summarized in Table 3.1-5.

Table 3.1-4. Elemental Solubility of Radionuclides in Near Field Concentrated Brine at 25°C

Element	Distribution Type	Solubility (molal)	Source
U	Triangular	4.89E-08 (min); 1.12E-07 (mode); 2.57E-07 (max)	Wang and Lee (2010)
Pu	Triangular	1.40E-06 (min); 4.62E-06 (mode); 1.53E-05 (max)	
Am	Triangular	1.85E-07 (min); 5.85E-07 (mode); 1.85E-06 (max)	
Np	Triangular	4.79E-10 (min); 1.51E-09 (mode); 4.79E-09 (max)	
Th	Triangular	2.00E-03 (min); 4.00E-03 (mode); 7.97E-03 (max)	
Tc	Log-triangular	4.56E-10 (min); 1.33E-08 (mode); 3.91E-07 (max)	
Sn	Triangular	9.87E-09 (min); 2.66E-08 (mode); 7.15E-08 (max)	
Ac, Cm	Constant	5.85E-07	Appendix C of this report
Cl	Constant	4.20	
Nb	Constant	1.60E-05	
Pa	Constant	1.51E-09	
Pd	Constant	4.00E-04	
Sb	Constant	6.30E-05	
Se	Constant	2.00E-05	
Zr	Constant	1.00E-10	
C, Cs, I, Ra, Sr	N/A	Unlimited solubility	

Table 3.1-5. Model Parameters for the Near-Field and Interface Region for the Reference Case of Salt GDS Model

Parameter	Distribution Type	Parameter Value and Description	Source
Near Field			
Thickness	Constant	1.56 m (equal to waste package diameter)	
Porosity (salt bedrock)	Log-uniform	0.01 (min); 0.1 (max)	Vaughn et al. (2000)
Density (salt bedrock)	Constant	2500 kg/m^3	
Porosity (degraded waste package)	Uniform	0.3 (min); 0.5 (max)	
Brine Flow Rate to Interface Rock Block (m/yr)	N/A	Sampled from 100 brine flow rate histories	Section 3.1.3 of this report
Radionuclide Sorption	N/A	Assume no sorption	
Radionuclide Solubility	N/A	Near-field solubility	Table 3.1-4 of this report
Interface Rock Block			
Thickness	Constant	5.0 m	
Porosity (salt bedrock)	Log-uniform	0.01 (min); 0.1 (max)	Vaughn et al. (2000)
Density (salt bedrock)	Constant	2500 kg/m^3	
Brine Flow Rate to Underlying Interbed (m/yr)	N/A	Sampled from 100 brine flow rate histories	Section 3.1.3 of this report
Radionuclide Sorption	N/A	Assume no sorption	
Radionuclide Solubility	N/A	Far-field solubility	Table 3.1-6 of this report

Table 3.1-6. Elemental Solubility of Radionuclides for Far-Field Dilute Brine at 25°C

Element	Distribution Type	Description (solubility in molal)	Source
U	Triangular	9.16E-05 (min); 2.64E-04 (mode); 7.62E-04 (max)	Wang and Lee (2010)
Pu	Triangular	7.80E-07 (min); 2.58E-06 (mode); 8.55E-06 (max)	
Am	Triangular	3.34E-07 (min); 1.06E-06 (mode); 3.34E-06 (max)	
Np	Log-triangular	1.11E-06 (min); 1.11E-05 (mode); 1.11E-04 (max)	
Th	Triangular	8.84E-06 (min); 1.76E-05 (mode); 3.52E-05 (max)	
Sn	Triangular	1.78E-08 (min); 4.80E-08 (mode); 1.29E-07 (max)	
Ac, Cm	Constant	5.85E-07	Appendix C of this report
Cl	Constant	4.20	
Nb	Constant	1.60E-05	
Pa	Constant	1.51E-09	
Pd	Constant	4.00E-04	
Sb	Constant	6.30E-05	
Se	Constant	2.00E-05	
Zr	Constant	1.00E-10	
C, Cs, I, Ra, Sr, Tc	N/A	Unlimited solubility	

3.1.2.7 Far Field

As discussed in Section 3.1.2.1, the reference case (the undisturbed scenario) assumes that an interbed below the repository is the major pathway for radionuclide release and transport from the repository, and this assumption is supported by the model results from WIPP (Helton et al. 1998). The interbed is assumed to be composed of a mixture of evaporite minerals (such as anhydrite) and clay, and is assumed to run horizontally in parallel with the repository (Figure 3.1-1). The interbed is assumed to be 1-m thick, with its width to be the same as that of repository; the interbed cross sectional area to water flow is the bed thickness times the width. The interbed features were adopted from the dominant underlying marker bed of the WIPP (Helton et al. 1998). As depicted in Figure 3.1-1, dissolved radionuclides are transported into the interbed over its length below the repository; this portion of the interbed is referred to as the repository interbed in the analysis.

The elemental solubilities applied to the far-field brine at 25°C in the salt GDS far-field interbed are shown in Table 3.1-6. As described in Section 3.1.2.6, these elemental solubilities are based on the data and calculation from Wang and Lee (2010) and in Appendix C of this report. Elements C, Ra, Sr and Tc are implemented as unlimited solubility in the far-field model because their solubility calculations have not been completed. Sorption of radionuclides on the interbed filling medium is modeled with an equilibrium Kd approach. The model parameters for radionuclide transport in the interbed for the reference scenario are listed in Table 3.1-7. Element Pb is implemented as nonsorbing in the interbed because analysis for its sorption behavior on the interbed filling materials has not been completed.

Table 3.1-7. Far-Field Model Parameters for Radionuclide Transport in the Underlying Interbed for the Reference Case of Salt GDS Model

Parameter	Distribution Type	Parameter Value and Description	Source
Thickness	Constant	1 m	Vaughn et al. (2000)
Porosity	Constant	0.01	
Density	Constant	2500 kg/m^3	
Brine Flow Rate (m/yr)	N/A	Sample from 100 time-dependent flow rate histories	Section 3.1.3 of this report
Longitudinal Dispersivity	Constant	10% of flow conduit length	
Kd for radioelements (mL/g):			
U	Uniform	0.2 (min); 1 (max)	Lappin et al. (1989); McKinley and Scholtis (1992); Muller et al. (1981); Tien et al. (1983)
Pu	Uniform	70 (min); 100 (max)	
Np	Uniform	1 (min); 10 (max)	
Am	Uniform	25 (min); 100 (max)	
Th	Uniform	100 (min); 1000 (max)	
Tc	Uniform	0 (min); 2 (max)	
Cs	Uniform	1 (min); 20 (max)	
Sr	Uniform	1 (min); 80 (max)	
Ac, Cm	Log-uniform	5 (min); 500 (max)	McKinley and Scholtis (1992) (Kd values reduced by a factor of 10 to account for the high salinity of brine.)
C	Uniform	0 (min); 0.6 (max)	
Nb, Pd	Constant	0.1	
Pa	Log-uniform	1 (min); 500 (max)	
Sb	Constant	10	
Se	Uniform	0.2 (min); 0.5 (max)	
Sn	Uniform	2 (min); 10 (max)	
Zr	Log-uniform	3 (min); 500 (max)	
Cl, I, Pb	Constant	0 (no sorption)	

The salt GDS model assumes that the interbed extends well beyond the repository boundary. Radionuclides are transported in the interbed by advection and diffusion to a distance of 5 km down-gradient from the edge of the repository, where it is assumed that contaminated brine is released to an aquifer and a “hypothetical” drinking water pumping-well (biosphere) withdraws water from the aquifer. This portion of the interbed is referred to as the far-field interbed in the analysis.

3.1.2.8 Biosphere Model

Radiation exposure, or dose, to a receptor in the biosphere is used as a performance metric for the all of the GDS analyses. The salt GDS model includes a hypothetical reference biosphere that is assumed to be located at 5-km down-gradient from the salt GDS boundary. The International Atomic Energy Agency’s (IAEA) BIOMASS Example Reference Biosphere 1B (ERB 1B) dose model (IAEA 2003) is used to convert the dissolved radionuclide concentrations in groundwater at a hypothetical drinking well location to an estimate of annual dose to a receptor based on drinking well water consumption. The ERB 1B is deliberately designed to be very simple, being focused on a simple biosphere system and single exposure pathway. It is characterized by a drinking water well bored through the overburden into an aquifer that has been contaminated by radionuclide releases from the repository. Previous experience from more comprehensive biosphere modeling studies has shown that a drinking water well may sometimes represent a significant or even, depending on other aspects of the assessment context, a dominant pathway for release and exposure (IAEA 2003). The ERB 1B dose model calculates dose to the receptor using Equations 4-27 through 4-30.

The model assumes a dilution rate of 1×10^4 m^3/yr in the aquifer and an individual water consumption rate of 1.2 m^3/yr (IAEA 2003). For the above dilution rate, the far-field interbed brine is assumed to be diluted to a potable level. It is assumed that recharge in the interbed and aquifer would sustain the well withdrawal rate for the full duration of the simulation. The ERB 1B parameters used to represent the salt GDS biosphere are provided in Table 3.1-8.

Table 3.1-8. IAEA ERB 1B Parameters for the Salt GDS Biosphere

Aquifer dilution rate: 1.00E+04 m^3/yr			
Well-water consumption rate: 1.2 m^3/yr			
ERB 1 Dose Coefficient			
Isotope	**Sv/Bq**	**Isotope**	**Sv/Bq**
^{227}Ac	0.00E+00	^{242}Pu	2.40E-07
^{241}Am	2.00E-07	^{226}Ra	2.17E-06
^{243}Am	2.01E-07	^{228}Ra	0.00E+00
^{14}C	5.80E-10	^{126}Sb	0.00E+00
^{36}Cl	9.30E-10	^{79}Se	2.90E-09
^{245}Cm	2.15E-07	^{126}Sn	4.70E-09
^{135}Cs	2.00E-09	^{90}Sr	3.07E-08
^{137}Cs	1.30E-08	^{99}Tc	6.40E-10
^{129}I	1.10E-07	^{229}Th	6.13E-07
^{93}Nb	0.00E+00	^{230}Th	2.10E-07
^{237}Np	1.11E-07	^{232}Th	1.06E-06
^{231}Pa	1.92E-06	^{232}U	0.00E+00
^{210}Pb	0.00E+00	^{233}U	5.10E-08
^{107}Pd	3.70E-11	^{234}U	4.90E-08
^{238}Pu	2.30E-07	^{235}U	4.73E-08
^{239}Pu	2.50E-07	^{236}U	4.70E-08
^{240}Pu	2.50E-07	^{238}U	4.84E-08
^{241}Pu	0.00E+00	^{93}Zr	1.22E-09

Source: IAEA 2003, Table C.5.

Note that applying the ERB 1B dose model at the boundary location is an arbitrary modeling choice to produce the uniform performance measure for comparative studies of the considered GDS options and does not indicate any realistic dose implications. In addition, the determination of the dose model parameter values and resulting dose conversion factors does not depend on the GDS, but rather on the biosphere beyond the GDS, the habits of the population in that biosphere, and potentially the regulatory framework. A variety of biospheres and local populations could be present over a given GDS and the resulting dose conversion factors may vary significantly. Therefore, the results presented in this report *should not* be construed as being indicative of the true performance of the GDS options or compared to any regulatory performance objectives regarding repository performance.

3.1.2.9 Disturbed Scenario Analysis

The salt GDS disturbed scenario is designed to analyze the impact of an atypical process that provides a fast pathway for radionuclide release to the far field and the effect of the far-field performance in response to the fast-pathway releases. The current salt GDS model uses a "stylized" human intrusion for the disturbed scenario (Figure 3.1-1). The scenario assumes that a single borehole penetrates a waste package and a pressurized brine reservoir below the repository at 1,000 yr after repository closure and provides a fast pathway for dissolved radionuclides to the overlying aquifer. In a "tight" repository environment, such as in a salt repository, waste packages are expected to be isolated by consolidated salt rock as a result of salt creep deformation, thus limiting the inventory available for release from the human intrusion scenario. To capture this effect, the number of waste packages affected (one penetrated plus, if any, neighboring packages affected) is randomly sampled between one and five (uniform distribution). This represents the total amount of waste inventory that becomes available for the fast pathway release by the human intrusion scenario.

The associated processes for the fast pathway release are specific to the geologic settings and features of a salt GDS. Unlike the reference (or undisturbed) scenario, the human intrusion scenario assumes that the waste packages that are affected remain intact until a borehole penetration occurs and that, once it has occurred, affected waste packages and waste form canisters inside the waste packages provide no barrier performance. The waste forms inside affected waste packages start to degrade when the human intrusion occurs (i.e., 1,000 yr after repository closure). This is a reasonable approach considering that the scenario is to analyze the impacts of a potential fast pathway for the affected inventory (typically much smaller than the reference scenario) and the far-field performance in response to the event. The modeling assumption will be refined as the model and analysis progress.

Dissolved radionuclides from the affected waste packages are carried upward through the borehole by pressurized brines from the repository and brine pocket, and released to an overlying carbonate aquifer. The steady-state brine flow rate through the borehole is sampled between 0.1 and 5.0 m^3/yr (uniform distribution). The overlying aquifer is assumed to comprise primarily dolomite matrix with clays dispersed in the matrix. The current human intrusion scenario does not consider the potential dose impacts of the waste that could be brought up directly to the surface as a result of the drilling activities as the analysis is designed to evaluate the impact of the geosphere and system responses to human intrusion. The model assumes that location of the borehole penetration in the repository is uncertain, and does not consider the distance from the penetration location to the repository boundary.

The mass of radionuclides released to the overlying aquifer are evaluated against the solubility for the far-field dilute brine (Table 3.1-6). If the concentrations of radionuclides exceed their solubility limits, the excess mass of the radionuclides precipitates out of the water and remains as a solid until it dissolves back to the water. The dissolved radionuclides are transported in the aquifer to a hypothetical drinking well location 5 km down-gradient from the repository boundary. Sorption of radionuclides on the aquifer filling medium is modeled with an equilibrium Kd approach. Table 3.1-9 lists key transport parameters and their values for the overlying aquifer. Element Pb is implemented as nonsorbing in the assumed carbonate aquifer because analysis for its sorption behavior on the aquifer filling materials has not been completed. As for the reference scenario analysis, the same hypothetical biosphere is assumed to exist at that location, and the reference biosphere model (IAEA ERB 1B model) (IAEA 2003) is applied to calculate the dose.

Table 3.1-9. Far-Field Parameters for Overlying Carbonate Aquifer for the Disturbed Scenario

Parameter	Distribution Type	Parameter Value and Description	Source
Aquifer Thickness	Constant	4 m	Lappin et al. (1989), Table E-6; Brush and Storz (1996)
Matrix Porosity	Uniform	0.07 (min); 0.3 (max)	
Bulk Density	Constant	2800 kg/m^3	
Matrix Tortuosity	Uniform	0.03 (min); 0.5 (max)	
Brine Flow Rate Upward through Borehole (m^3/yr)	Uniform	0.1 (min); 5.0 (max)	Helton et al. 1998
Aquifer Water Flow Rate (m/yr)	Log-uniform	3.15E-03 (min); 3.15E+01 (max)	Helton et al. (1998), Figure 12.1.1
Longitudinal Dispersivity	Constant	10% of flow conduit length	
Kd for radioelements (mL/g):			
U	Uniform	0.03 (min); 20 (max)	Brush and Storz (1996); Muller et al. (1981); Pepping et al. (1983); Tien et al. (1983)
Pu	Log-uniform	20 (min); 1.0E+04 (max)	
Np	Log-uniform	1 (min); 200 (max)	
Am	Uniform	20 (min); 400 (max)	
Th	Log-uniform	7.0E+02 (min); 1.0E+04 (max)	
Tc	Triangular	0 (min); 50 (mode); 100 (max)	
Cs	Triangular	40 (min); 500 (mode); 3000 (max)	
Sr	Triangular	5 (min); 13 (mode); 4.0E+04 (max)	
I	Uniform	0.01 (min); 100 (max)	
Ac, Cm	Log-uniform	100 (min); 1.0E+05 (max)	McKinley and Scholtis (1992)
C	Log-uniform	1.0E-04 (min); 2000 (max)	
Nb	Constant	10	
Pa	Log-uniform	10 (min); 1000 (max)	
Pd	Uniform	4 (min); 100 (max)	
Sb	Constant	100	
Se	Uniform	1 (min); 8 (max)	
Sn	Log-uniform	50 (min); 700 (max)	
Zr	Log-uniform	10 (min); 8300 (max)	
Cl, Pb	Constant	0 (no sorption)	

3.1.3 Brine Flow Analysis

Once heat-generating UNF and/or HLW are emplaced in a salt repository, it is likely that moisture in the surrounding materials will be driven out by the heat, forming a dry-out region around the waste (Hansen and Leigh 2011). This section documents an analysis that was conducted to evaluate how long this dry-out region around the waste could persist and to estimate brine flow rate out of the waste disposal area and in the underlying interbed. The brine flow rates resulting from this analysis are abstracted and input to the salt GDS analysis.

3.1.3.1 Approach

The BRAGFLO software (Nemer 2007) is currently used to model the brine and gas flow in and around the WIPP. BRAGFLO models two phase flow through porous media and includes the effects of many other processes such as gas generation from iron corrosion and rock compressibility. BRAGFLO was used to evaluate the persistence of the dry-out region in this analysis.

The NUTS software (Gilkey 2006) simulates the transport in and around the WIPP. NUTS draws on the flow fields determined by BRAGFLO and utilizes a tracer to track the flow of the fluid of interest. NUTS was used to determine the brine flow from the waste package to the surroundings and to determine the portion of the brine that has contacted waste.

3.1.3.2 Model Geometry

The initial geometry for the brine flow analysis is a 6 m by 6 m by 12 m alcove completely filled with 38% porosity crushed salt and a 1.6 m diameter, 5.5 m length waste package placed against the back wall (Figure 3.1-2). After the placement of the waste package in the alcove, it is assumed that the crushed salt dries out due to the elevated temperatures and subsequently reconsolidates to a final porosity of 1%. This is reasonable given the rapid consolidation time relative to repository timeframes. Elevated temperatures would increase the consolidation process (Hansen and Leigh 2011). Taking into account the reconsolidation of the crushed salt and the creep of the surrounding salt rock, the final alcove dimensions were determined to be 4.8 m by 4.8 m by 12 m, assuming that the length of the alcove remained the same (Figure 3.1-2). To convert the waste package dimension to rectangular coordinates, the 1.6-m diameter waste package was approximated as a 1.4-m by 1.4-m rectangular waste package to preserve the volume of the waste package.

As the alcove is mined out, the surrounding rock is disturbed. The depth of the disturbed zone was estimated by approximating the stress trajectories around the alcove and determining the maximum distance between the stress trajectories and the alcove walls. Drawing a circle that connects the four corners of the 6 m by 6 m alcove to represent the stress trajectories gives a maximum distance between the circle and the edge of the alcove of 1.24 m. This depth was then multiplied by 135% to account for

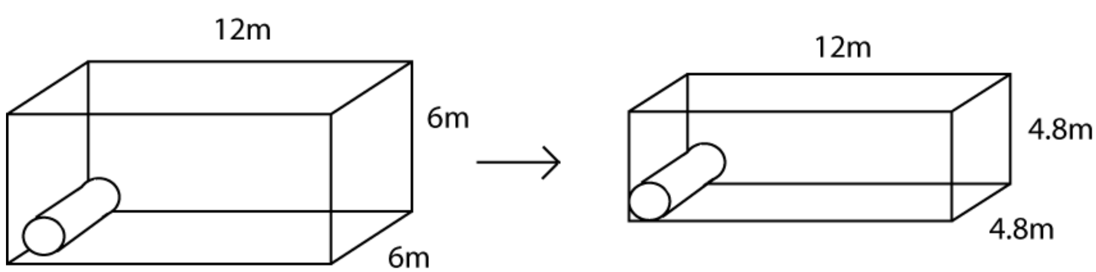


Figure 3.1-2. Illustration of Initial and Final Alcove Geometry

surrounding intact rock that may have been disturbed by the drying, heating or reconsolidation processes. The moisture from the disturbed zone is also assumed to be driven out by the elevated temperatures. The disturbed zone is assumed to be completely reconsolidated at the commencement of the calculation resulting in a dry intact salt material. This is reasonable given the rapid reconsolidation time relative to repository timeframes. For this analysis, the alcove was placed in the center of a salt bed with a 260 m vertical dimension and 1,035 m horizontal dimension, with impermeable layers both above and below the salt bed. A horizontal anhydrite layer (interbed) was connected to the lower disturbed zone. The boundaries were selected to be far enough away from the alcove so as not to influence the calculations near the alcove over the duration of the numerical simulation.

The primary objective in creating the modeling grid is to capture the effects of potential brine flow into the initial dry-out region. This can be accomplished by using a vertical two-dimensional (2D) grid, oriented along the length of the alcove (Figure 3.1-3). The grid is shown as a logical grid in Figure 3.1-3, with the length (Δx), width (Δz) and height (Δy) of each grid cell indicated (in meters). A technique of "radial flaring" was used to capture three-dimensional (3D) flow effects. The width of each grid cell increases with distance away from the center of the alcove, simulating the convergent or divergent flow centered on the alcove.

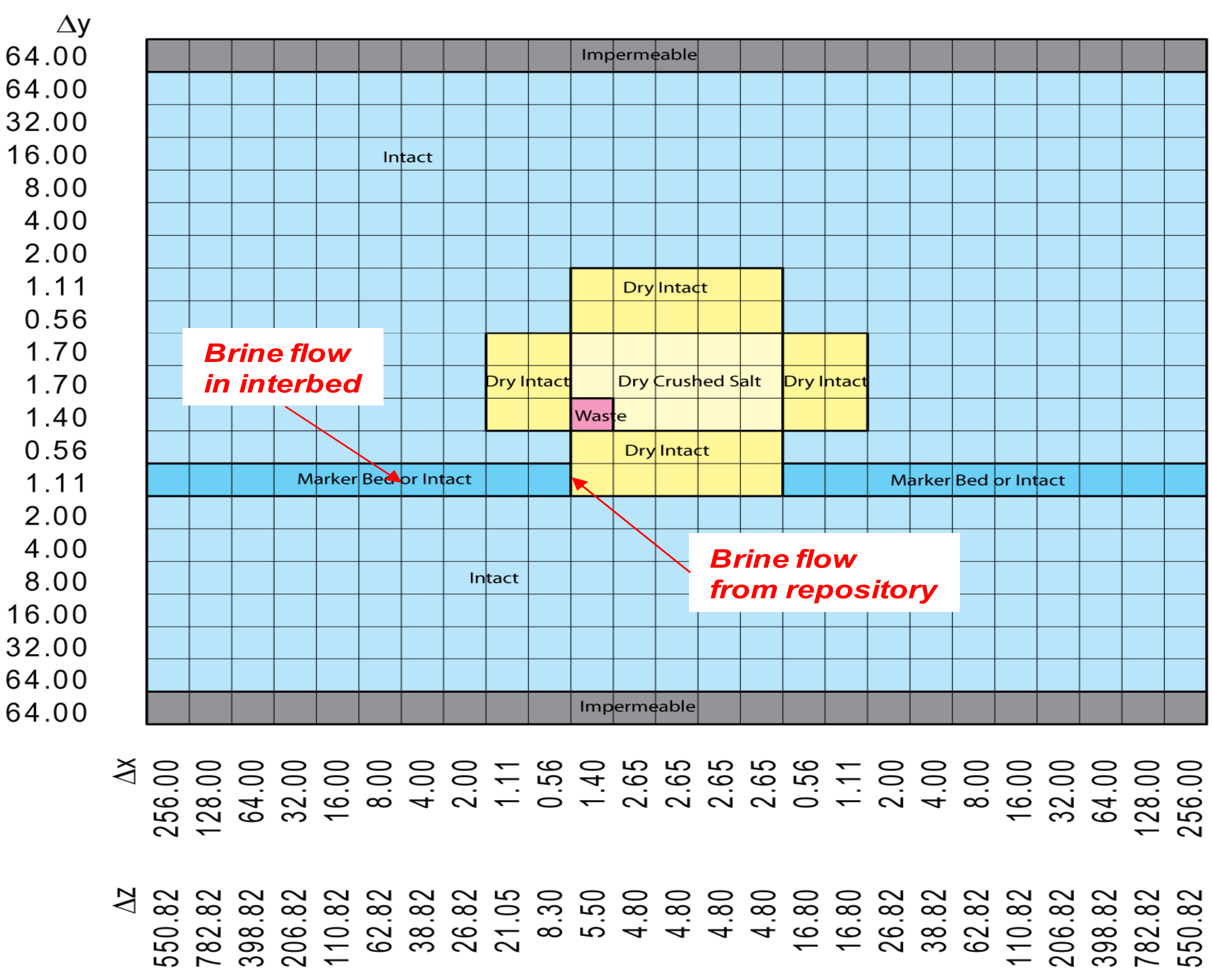


Figure 3.1-3. Long-term Brine Flow Grid Used in Analysis

The resulting grid contains six different materials: (1) impermeable (gray); (2) saturated intact salt (light blue); (3) dry intact salt (yellow); (4) dry reconsolidated crushed salt (light yellow); (5) waste material (pink); and (6) interbed (or marker bed) (blue). The properties of an anhydrite layer were used for the interbed material.

Two locations were selected to obtain for the brine velocity information for use in developing the abstraction to be used in the salt GDS (Figure 3.1-3): (1) brine velocities from the repository chosen at the edge of the initial dry-out region right below the waste disposal area; and (2) brine velocities in the underlying interbed chosen at 8 m from the edge of initial dry-out region. The 8-m brine velocities were used for the far-field interbed brine velocities. This is conservative because brine velocities are expected to decrease with the distance from the repository due to increased spread-out of brines with distance and associated pressure drop.

3.1.3.3 Initial Conditions

The initial conditions were chosen to represent a dry, low pressure state for the alcove and waste material, with a saturated, high pressure state for the surrounding formation. The initial brine pressures in the dry-out regions and waste package were set to a range from atmospheric to lithostatic pressure. The waste package was set to initially be completely dry (0% brine saturation), while the dry-out regions were given a range of initial brine saturations from 0.15% to 10%. A range was used so that the sensitivity of the results to the initial pressure and brine saturation of the dry-out region could be determined. For the impermeable, intact salt and interbed materials, the initial brine pressures were set to correspond to the lithostatic pressure, which is based on the relative depth, and initial brine saturations were set to 100%, which is consistent with the characterization of intact salt. The initial amount of iron present in the alcove was determined by assuming that the outer 0.05 m of the waste package was iron. A 1.6-m outer diameter, 5.5-m long, 0.05-m thick annulus of iron would contain 1.34 m^3 of iron. Using a density of 7,870 kg/m^3, the total initial mass of iron (10,500 kg) was calculated. For the brine outflow tracer calculations, an initial tracer concentration of 1 kg/m^3 was used in the waste area. This is somewhat arbitrary as contaminated brine concentrations will be determined relative to this initial tracer concentration.

3.1.3.4 Model Parameters

There is a significant amount of uncertainty associated with characterizing the physical properties of geologic materials. Properties such as permeability and porosity are usually measured indirectly and can vary significantly depending on location. This uncertainty is dealt with by running multiple realizations in which the values of uncertain parameters are varied. For this analysis, a range of values were used for 19 parameters (Table 3.1-10). The LHS software (Vugrin 2006) was used to create 100 distinct parameters sets that span the full range of parameter uncertainty.

The properties used for the impermeable, intact salt and interbed materials in this analysis correspond to the properties used in the WIPP analysis (Clayton 2010). The dry intact salt and dry reconsolidated crushed salt material properties were aligned with the intact salt material properties, except the permeability was increased by a factor of one thousand. The ranges of the initial pressure and saturation of the dry-out region, the waste material permeability and porosity, and the iron corrosion rate were chosen to be able to determine the sensitivity of the results to these input values. The iron corrosion rate was converted from a corrosion depth rate to a volumetric rate by multiplying by the waste package surface area times a 1.2 factor intended to account for surface roughness.

Table 3.1-10. Ranges and Distributions Used for Uncertain Parameters

Parameter	Lower Bound	Upper Bound	Distribution Type	Unit
Intact Salt Permeability	1.0E-24	1.0E-21	Log-uniform	m^2
Intact Salt Porosity	0.001	0.0519	Log-uniform	none
Intact Salt Compressibility	3.0E-12	2.0E-10	Log-uniform	Pa^{-1}
Relative Permeability Model	vGP	BC	50/50 split	none
Dry Intact Salt Permeability	1.0E-21	1.0E-18	Log-uniform	m^2
Dry Intact Salt Porosity	0.001	0.0519	Log-uniform	none
Dry Intact Salt Compressibility	3.0E-12	2.0E-10	Log-uniform	Pa^{-1}
Dry Crushed Salt Permeability	1.0E-21	1.0E-18	Log-uniform	m^2
Dry Crushed Salt Porosity	0.001	0.0519	Log-uniform	none
Dry Crushed Salt Compressibility	3.0E-12	2.0E-10	Log-uniform	Pa^{-1}
Initial Pressure of Dry-out Region	1.01E+05	1.48E+07	Uniform	Pa
Initial Saturation of Dry-out Region	0.015	0.1	Uniform	none
Interbed Permeability	1.0E-21	1.0E-17	Log-uniform	m^2
Interbed Porosity	0.006	0.017	Uniform	none
Interbed Lambda	0.5	0.85	Uniform	none
Interbed Residual Brine Saturation	0.005	0.2	Log-uniform	none
Waste Material Permeability	1.0E-15	1.0E-12	Log-uniform	m^2
Waste Material Porosity	0.01	0.05	Uniform	none
Waste Package Iron Corrosion Rate	3.17E-16	3.17E-14	Log-uniform	m/s

3.1.3.5 Analysis Results and Brine Flow Rate Abstraction

The analysis is to evaluate the persistence of the dry, low pressure region surrounding the waste package. It also analyzed the amount of brine that enters the dry-out region from the surrounding formations, the pressure in dry-out region, and the amount of brine that exits the dry-out region. The final results for the brine outflow rate histories were abstracted for each of the 100 distinct parameters sets, and input to the salt GDS analysis. The analysis results are summarized as follows:

- Brine flow into the dry-out region begins as early as approximately 1 yr, with all parameter sets showing brine inflow by about 100 yr. Some of the parameter sets show up to 29 m^3 of brine entering the dry-out area, with the majority indicating that on the order of ~3 m^3 of brine enters the dry-out region after about 1,000 yr.
- As brine enters the dry-out region, it can react with the iron in waste package, causing it to corrode and produce gas. The brine inflow and gas production trigger an increase in the pressure in the dry-out region. The pressure in the dry-out region begins to increase as early as about 1 yr, with the majority of the parameter sets showing an increased pressure by 1,000 yr. The pressures at 1,000,000 yr can be near the surrounding lithostatic pressure of 14.8 MPa at repository elevation.
- When the pressure in the dry-out region is above the surrounding pressure, there is flow out of the dry-out region. Brine flow out of the dry-out region begins as early as ~100 yr. The total brine flow out of the dry-out region is 3 to 4 times less than the total brine flow into the dry-out region. Some brine is consumed during the generation of gas by corrosion.

- Not all of the brine that flows into the dry-out region contacts the waste and dissolves radionuclides. Likewise, not all of the brine that flows out of the dry-out region boundary has contacted the waste and is contaminated with dissolved radionuclides. In order to estimate the flow rate of contaminated brines flowing out of the dry-out region, a tracer with a unit concentration was applied to the brine in the waste disposal area. Then the maximum concentration of the tracer outside of the dry-out region was determined as a function of time. The analysis showed that the tracer concentration is significantly delayed and decreases with distance, and that the contaminated brine from the waste disposal area is limited to the immediate area of the dry-out region. The majority of the brine that flows out of the dry-out region has not mixed with the waste disposal area brine.
- The analysis showed that interbed permeability is the only interbed property to which the results are noticeably sensitive. The analysis results also showed that the main driver for brine flow is the pressure gradient and more than sufficient brine enters the dry-out region to saturate and pressurize the dry-out region between 1 and 1,000 yr.

The time-dependent velocity of the contaminated brine flowing out the repository and interbed was determined and used in the salt GDS performance analysis. This was determined by dividing the volumetric brine flow out of the dry region by the projected area of the pores, all multiplied by the concentration of the tracer. The projected area of the pores was calculated as the area of the grid cell perpendicular to the brine flow times the porosity of the interbed.

Figure 3.1-4 shows the results of the brine velocity histories from the repository and underlying interbed that are abstracted into the salt GDS model. For each location, a set of 100 flow rate histories (or 100 realizations) were calculated to represent the uncertainty in the brine flow rate that is derived from the

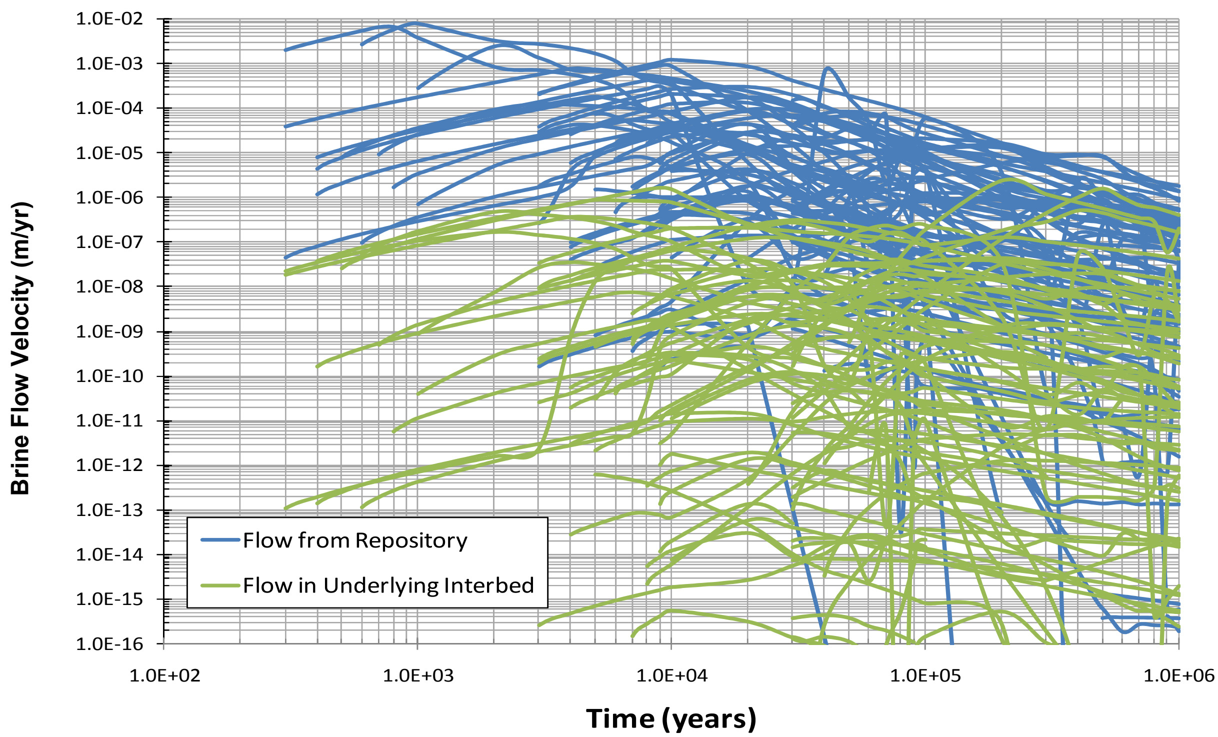


Figure 3.1-4. Abstraction Results for Brine Flow Rate Histories from the Repository and in Underlying Interbed

input parameter uncertainties (Table 3.1-10). The velocities are lower the further from the dry-out region due to the dilution of the surrounding uncontaminated brine. As the brine flow rates are very low for most of the realizations, especially in the interbed, radionuclide release and transport from a salt GDS would be dominated by diffusion as discussed in the model demonstration (Section 3.1.4).

The flow rate histories are implemented in the salt GDS model as a look-up table. The histories are sampled randomly in the GDS performance analysis, having the histories at the two locations perfectly correlated.

3.1.4 Model Demonstration

This section discusses analysis of the capability demonstration for the current version of the salt GDS model. The model results are presented in terms of the mean radionuclide mass release rate from the near field and far field as the intermediate metrics of performance, and the mean annual dose (mrem/yr) by individual radionuclide at the hypothetical accessible environment. The current model is part of an on-going effort to develop the capability of modeling the repository performance of a nuclear waste repository located in a generic salt host rock. Further improvements and refinements will be made as information from other UFD work packages (e.g., Natural System, EBS) matures. These further improvements and technical detail will be implemented in the GPAM described in Section 4 rather than in the salt GDS model, which will be retired. The use of the mean annual dose is an arbitrary choice to present and discuss the analysis results in order to facilitate a consistent and useful comparison among GDS options. The scientific basis for the results presented is immature, therefore *should not* be utilized for decision making at this time. The purpose remains a demonstration of modeling capability and as such represents a first look at viability. As the pedigree of the baseline matures, use for decision analysis, GDS option screening, and regulatory comparisons will be appropriate and remains a future goal.

The salt GDS model was implemented in GoldSim (GoldSim Technology Group 2009). The model demonstration was performed probabilistically, with 100 realizations for each case and over a time period of 1,000,000 yr.

3.1.4.1 Reference Scenario Analysis

This subsection discusses the model results for the reference scenario. Two repository waste inventory cases are considered for the analysis. For the reference scenario (undisturbed scenario), the waste inventory for Case 1 comprises the commercial UNF and DHLW. The waste inventory for Case 2 comprises the DHLW and hypothetical CHLW of the commercial UNF. As discussed in Section 3.1.2.2, the following assumptions are made for the hypothetical CHLW: (1) Ninety nine percent (99%) of uranium and plutonium are recovered from the commercial UNF inventory, and all others including transuranic elements and fission products remain in the waste stream; (2) CHLW contains the same radionuclides as in the DHLW; and (3) CHLW is encapsulated in borosilicate glass at the same radionuclide mass loading as for the DHLW.

Waste Inventory Case 1 takes a square repository footprint with a side of 3,270 m for disposal of a total of 37,157 waste packages (32,154 commercial UNF waste packages plus 5,003 DHLW waste packages) (Section 3.1.2.2). Inventory Case 2 needs a smaller square repository footprint with a side of 1,615 m for a total of 9,058 waste packages (5,003 DHLW waste packages plus 4,055 CHLW waste packages) (Section 3.1.2.2).

3.1.4.1.1 Waste Inventory Case 1

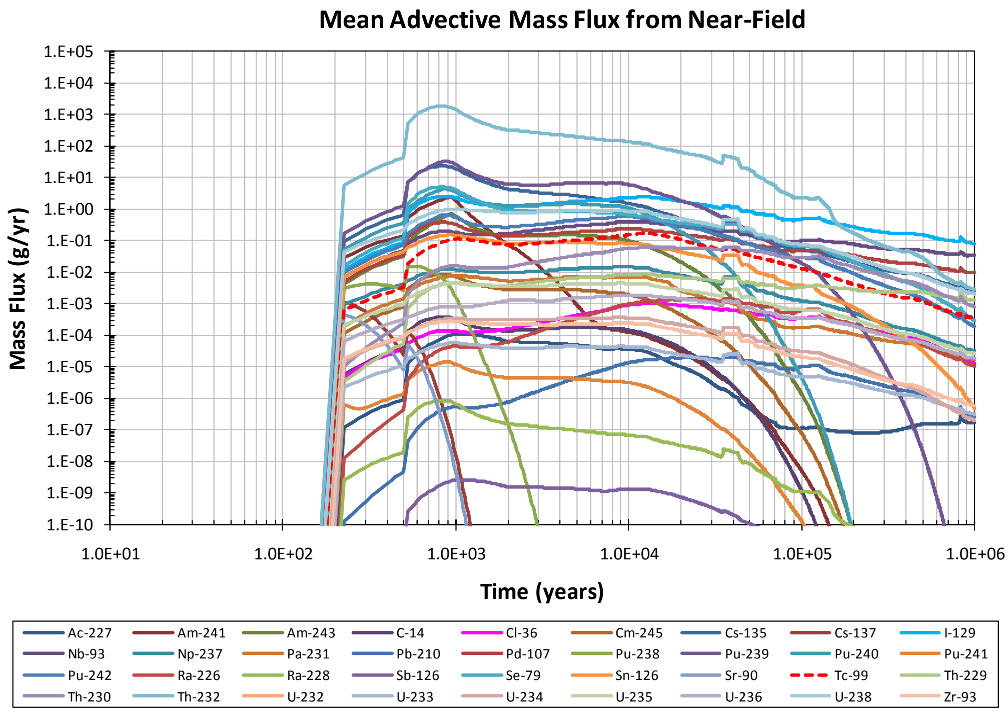
Figure 3.1-5 shows the model results for the mean advective and diffusive radionuclide mass release rate from the repository for Waste Inventory Case 1 (commercial UNF plus DHLW) of the reference scenario. As expected from the very low calculated brine flow rates from the repository (Figure 3.1-4), the release rates are dominated by diffusion and contribution from advection are negligible. As discussed in Section 3.1.2.6, sorption of radionuclides is not considered in the near field and interface rock below repository, so even these releases are over-estimated. ^{232}Th shows the highest mean release rate by both diffusion and advection, followed by ^{239}Pu and ^{135}Cs. The mean release rate of ^{129}I (nonsorbing, mobile radionuclide with unlimited solubility and a very long half-life) becomes important at later times (after about 10^5 yr). The broken curves shown for some radionuclides (e.g., ^{237}Np, ^{210}Pb, ^{226}Ra, ^{228}Ra, etc.) in the bottom figure are due to the back-diffusion (negative mass flux) and the inability to present negative values on a log plot.

Figure 3.1-6 shows the mean advective and diffusive release rates from the underlying interbed at the boundary of the repository footprint. Consistent with the conceptual model, radionuclides are transported into the underlying interbed over its entire length that underlies the repository (see Section 3.1.2.1 for the conceptual model discussion). As for the release from the repository, the mean diffusive release rate is much greater than the mean advective release rate. Sorption of radionuclides on the interbed filling materials is considered in the interbed, and ^{129}I (nonsorbing and unlimited solubility) becomes the dominant radionuclide released.

Figure 3.1-7 shows the mean advective and diffusive release rates from the far-field interbed at 5 km from the edge of the repository. Transport of radionuclides in the far-field interbed is similarly dominated by diffusion and is greatly retarded by sorption on the interbed filling materials. The calculated mean release rates are so low that there would be no meaningful consequence for the repository performance under this scenario and for this waste inventory case. This is demonstrated by the negligibly small mean annual dose at the hypothetical accessible environment shown in Figure 3.1-8.

3.1.4.1.2 Waste Inventory Case 2

Compared to Waste Inventory Case 1 (commercial UNF plus DHLW), Waste Inventory Case 2 (DHLW plus hypothetical CHLW) requires a smaller number of waste packages (9,058 waste packages vs. 37,157 waste packages) and one-fourth of the repository footprint area. This in turn results in a smaller volume of near field and available near-field water, and higher concentrations of soluble radionuclides (such as ^{129}I) in the near-field water provided solubility limits are not exceeded. Because of the assumptions made for the hypothetical CHLW (Section 3.1.2.2), the fission products inventory on a per-waste package basis is higher than that for Waste Inventory Case 1. For example, each CHLW waste package contains about 7,500 g of ^{129}I, which is about eight times greater than the per-waste package inventory mass of the radionuclides of commercial UNF. In addition, the fractional degradation rate of glass waste form (a mean rate of 4.9×10^{-4} per year) for the DHLW and CHLW is greater than the UNF degradation rate (a mean rate of 1.5×10^{-7} per year) (Section 3.1.2.5), releasing a greater amount of radionuclides into the near-field water per unit time. Note that both the DHLW and CHLW do not have ^{36}Cl inventory as discussed in Section 3.1.2.2. The fuel cycle inventory analysis reports zero inventory for ^{36}Cl for the DHLW (Carter and Luptak 2010), and the analysis is currently under review to confirm the ^{36}Cl inventory.



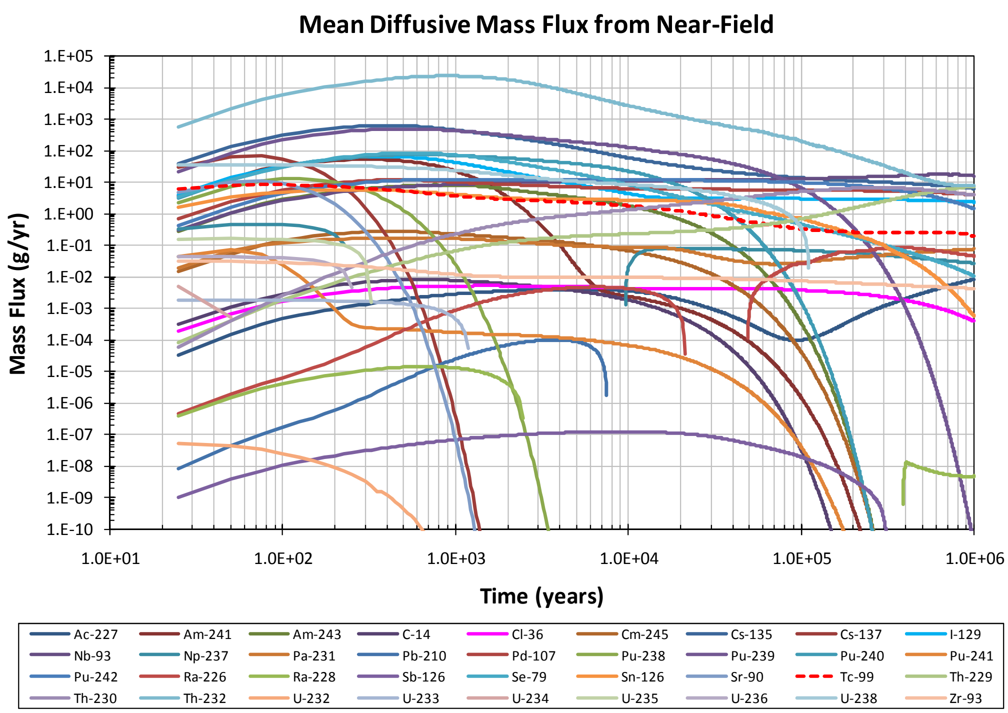


Figure 3.1-5. Model Results for Waste Inventory Case 1 of the Reference Scenario: Mean Advective and Diffusive Release Rate from Repository

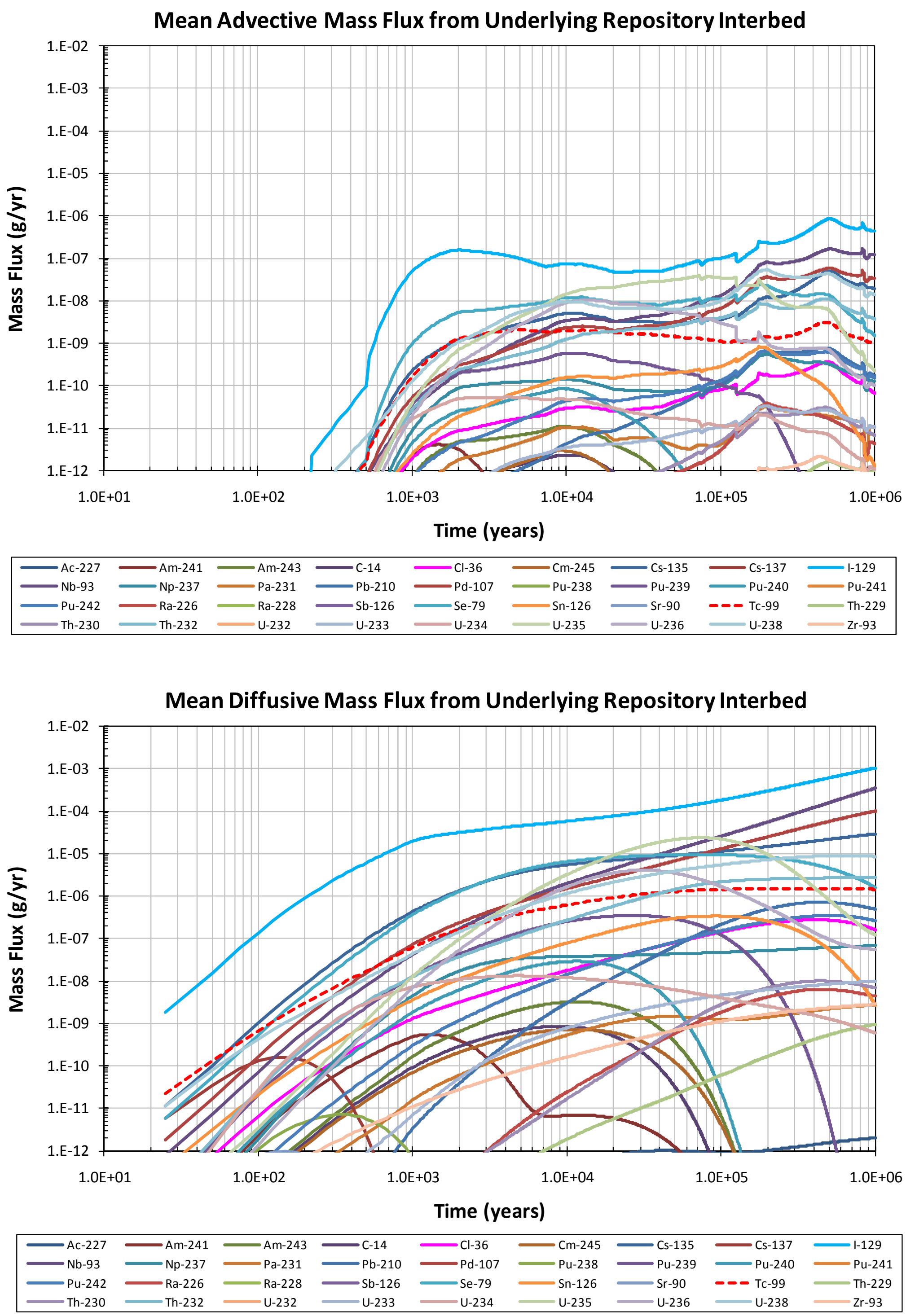
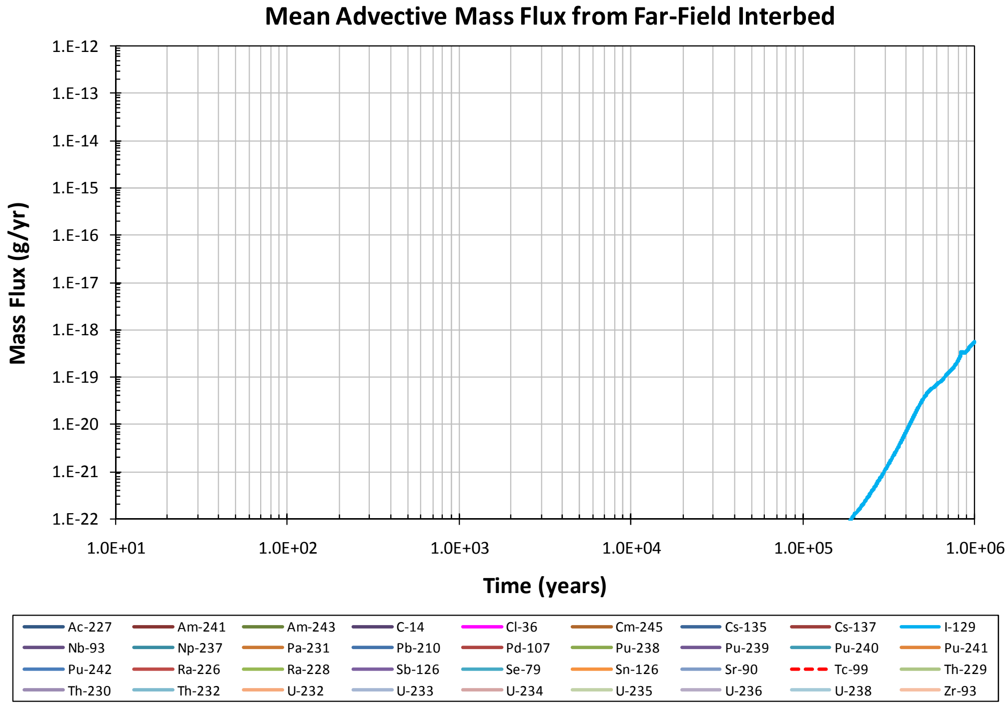


Figure 3.1-6. Model Results for Waste Inventory Case 1 of the Reference Scenario: Mean Advective and Diffusive Release Rate from the Underlying Interbed at the Boundary of Repository Footprint



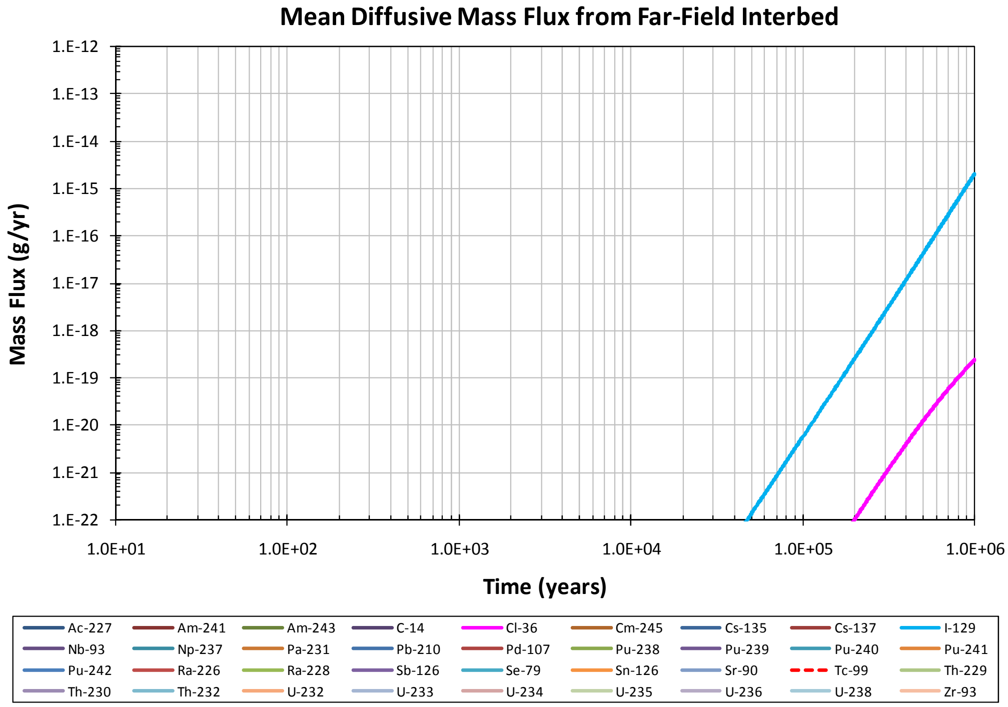


Figure 3.1-7. Model Results for Waste Inventory Case 1 of the Reference Scenario: Mean Advective and Diffusive Release Rate from the far-Field Interbed at 5 km from the Boundary of Repository Footprint

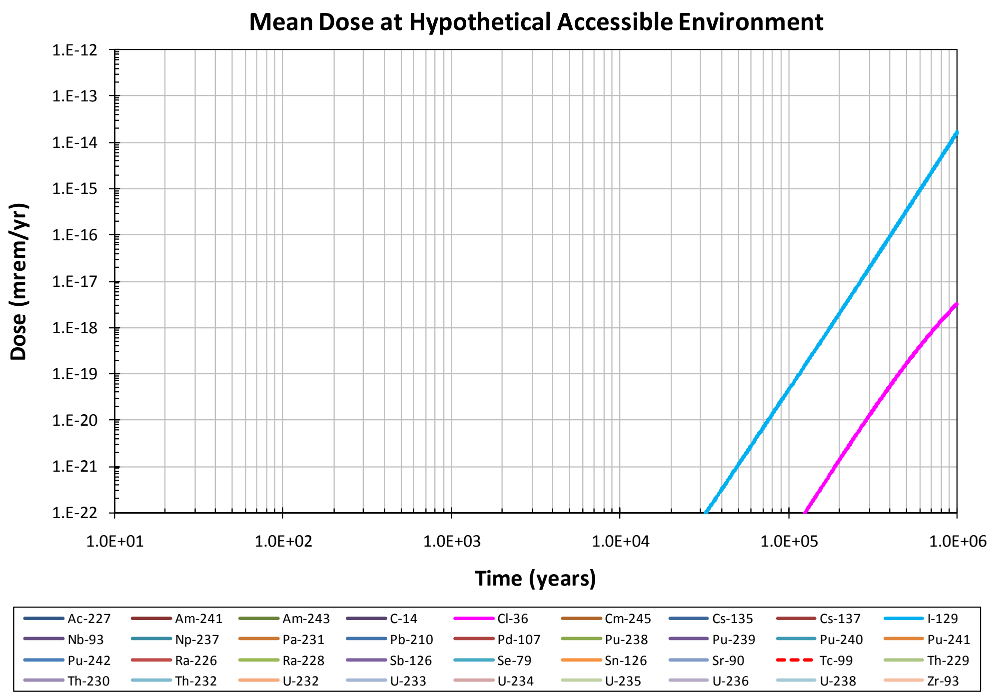
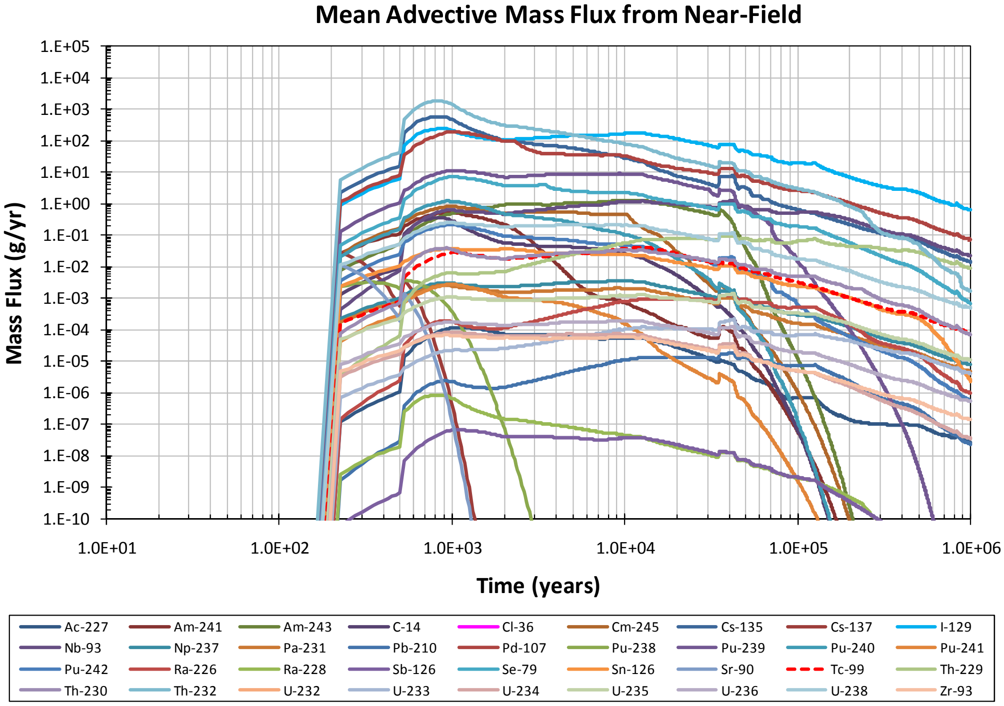


Figure 3.1-8. Model Results for Waste Inventory Case 1 of the Reference Scenario: Mean Annual Dose at the Hypothetical Accessible Environment at 5 km from the Boundary of Repository Footprint

Figure 3.1-9 shows the mean advective and diffusive radionuclide mass release rate from the repository for Waste Inventory Case 2 of the reference scenario. Again the diffusive releases are much greater than the advective releases. ^{232}Th is the dominant radionuclide in terms of the release rate from the repository at early time, followed by ^{135}Cs, ^{107}Pd, ^{129}I and ^{239}Pu. ^{229}Th becomes the dominant radionuclide after about 3×10^5 yr. The broken curves shown for some radionuclides in the diffusive release rate figure are due to the back-diffusion (negative mass flux). Compared to the repository release rates for Waste Inventory Case 1 (Figure 3.1-5), the release rates for Waste Inventory Case 2 are higher as the individual radionuclide curves are shifted higher, although the dominant radionuclide (^{232}Th) release rate remains about the same as its dissolved concentration is limited by the solubility.

Figure 3.1-10 shows the mean advective and diffusive release rates from the underlying interbed at the edge of the repository. The mean diffusive release rate is much greater than the mean advective release rate. Because sorption of radionuclides on the interbed filling materials is modeled for the interbed, ^{129}I (nonsorbing and unlimited solubility) becomes the dominant radionuclide in terms of the mean release rate from the interbed. Its release rates are one to two orders of magnitude greater than calculated for the Waste Inventory Case 1 because of the factors discussed above (greater inventory and higher waste form degradation rate).

Figure 3.1-11 shows the mean advective and diffusive release rates from the far-field interbed at 5 km from the boundary of repository footprint. Diffusive transport of radionuclides in the far-field interbed is greatly retarded by sorption on the interbed filling materials. Because it does not sorb, ^{129}I is the single dominant radionuclide in terms of the mean release rate, but its calculated mean release rates are still negligibly small. Because of the very low release rate of ^{129}I, there would be no meaningful consequence for the repository performance under this scenario and for this waste inventory case. This is shown by the calculable, but negligibly small mean annual dose by the radionuclide at the hypothetical accessible environment (Figure 3.1-12).



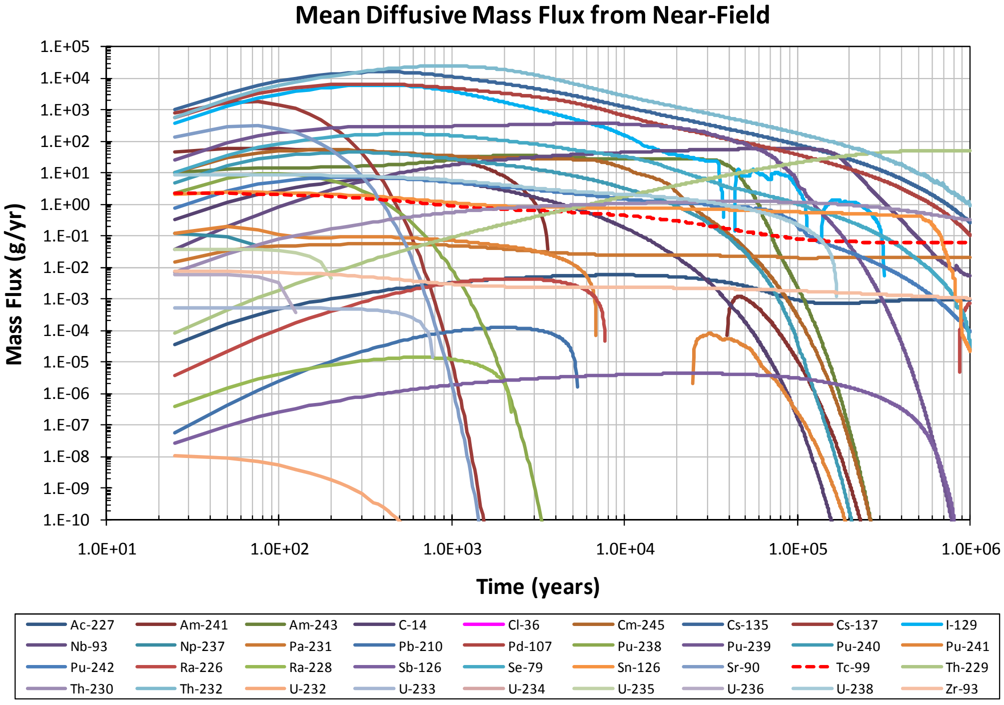
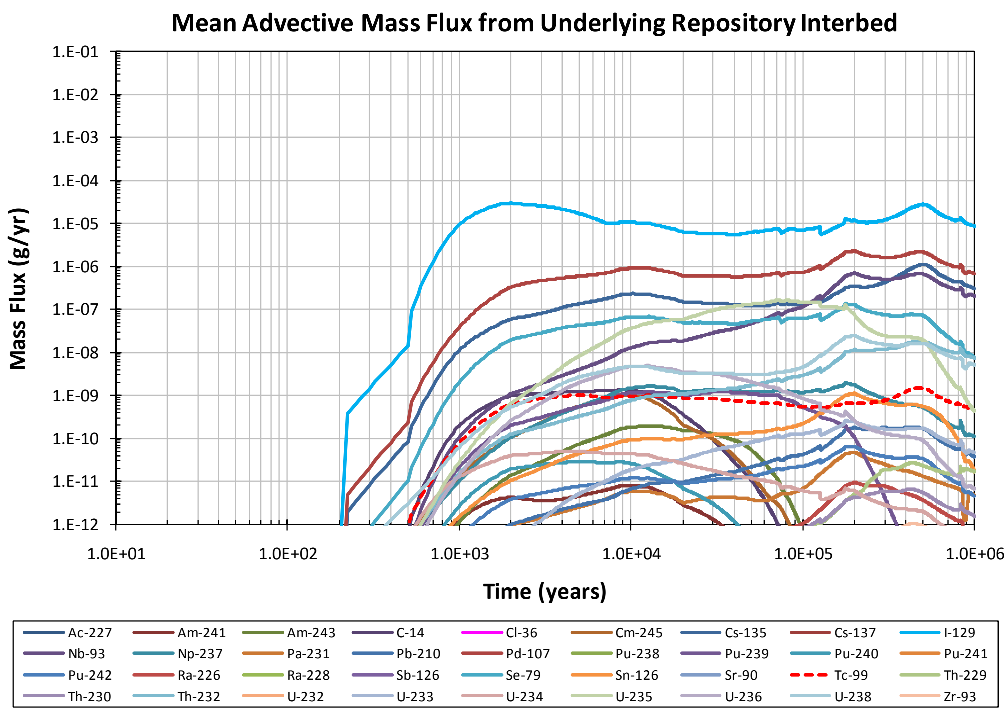


Figure 3.1-9. Model Results for Waste Inventory Case 2 of the Reference Scenario: Mean Advective and Diffusive Release Rate from Repository



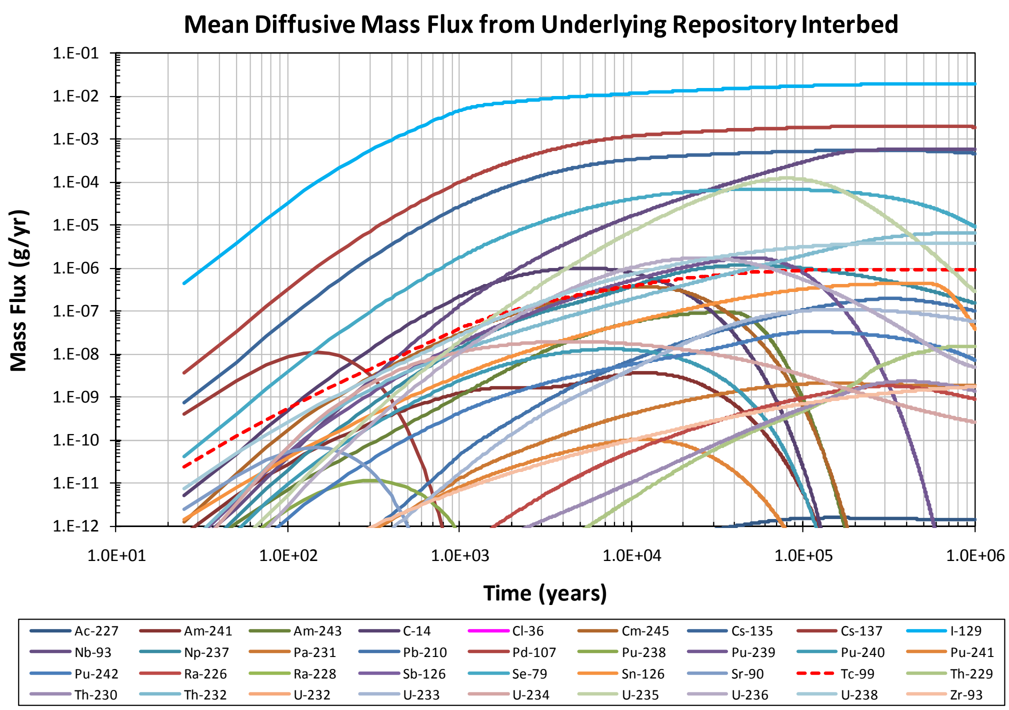
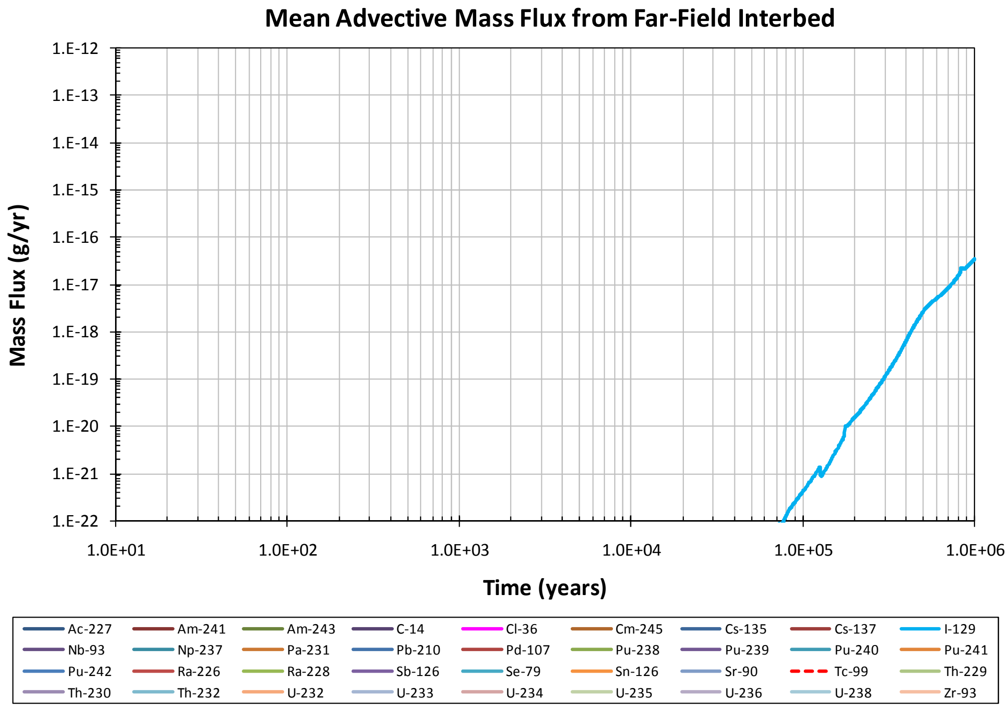


Figure 3.1-10. Model Results for Waste Inventory Case 2 of the Reference Scenario: Mean Advective and Diffusive Release Rate from the Underlying Interbed at the Boundary of Repository Footprint



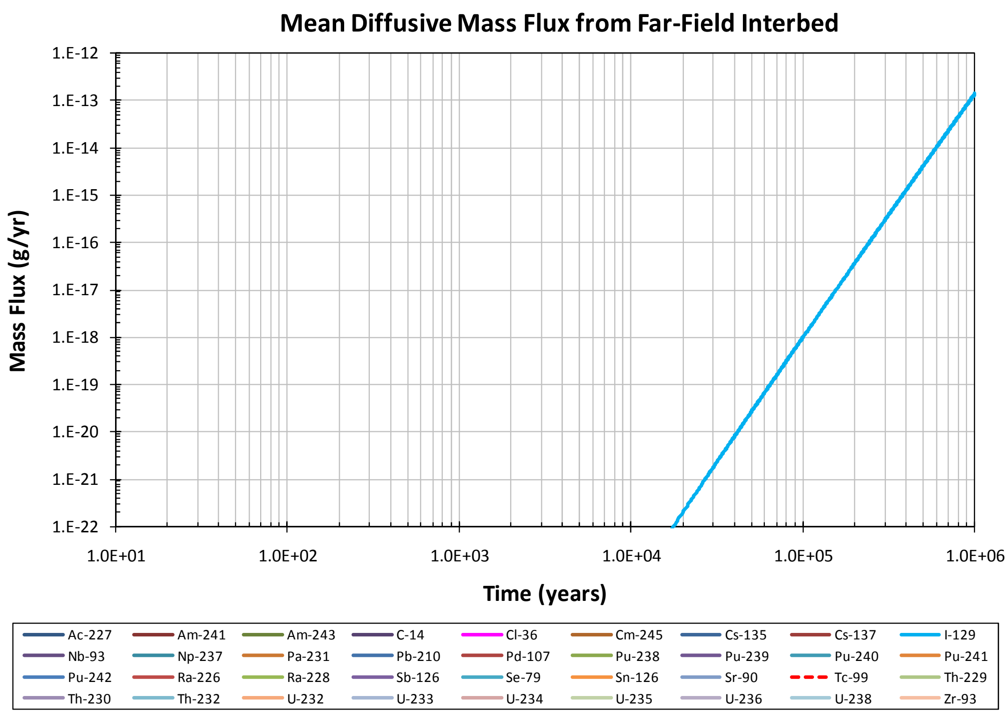


Figure 3.1-11. Model Results for Waste Inventory Case 2 of the Reference Scenario: Mean Advective and Diffusive Release Rate from the Far-Field Interbed at 5 km from the Boundary of Repository Footprint

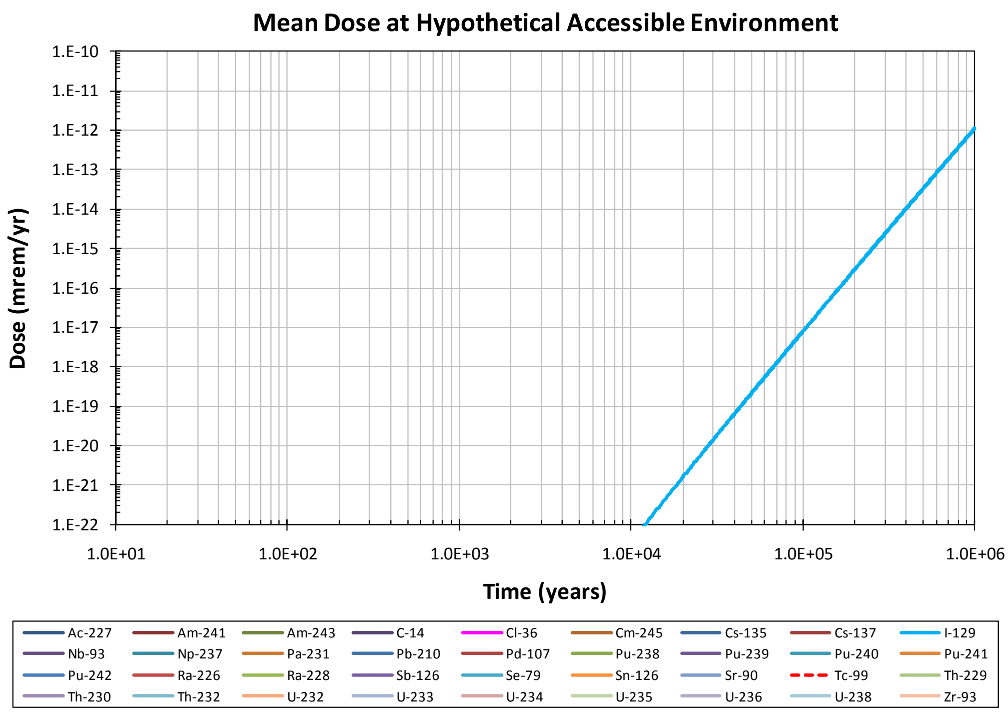


Figure 3.1-12. Model Results for Waste Inventory Case 1 of the Reference Scenario: Mean Annual Dose at the Hypothetical Accessible Environment at 5 km from the Boundary of Repository Footprint

3.1.4.2 Human Intrusion Scenario Analysis

Similar to the reference (or nominal) scenario analysis, two waste inventory cases are analyzed for the disturbed (or human intrusion) scenario analysis. For simplification, Waste Inventory Case 1 considers the situation in which only the commercial UNF waste packages are affected by the human intrusion activity; for Waste Inventory Case 2, only the DHLW waste packages are affected. Consistent with the conceptual model discussed in Section 3.1.2.1, the dissolved radionuclides that are released from the affected waste package(s) into the near-field water are transported upward by pressurized brine from the underlying pressurized brine reservoir through a borehole and released directly to the overlying aquifer. The aquifer water flow rate is several orders of magnitude greater than the brine flow rate in the interbed, and the radionuclides are transported advectively at much greater rates (Table 3.1-9 and Figure 3.1-4). The model assumes that the location of the borehole penetration in the repository is uncertain and does not consider the distance from the penetration location to the repository boundary. Refer to Section 3.1.2.9 for the human intrusion scenario discussion.

3.1.4.2.1 Waste Inventory Case 1

Figure 3.1-13 shows the model results of the mean mass release rate from the repository through a borehole that has penetrated the repository at 1,000 yr after repository closure. The release rate is at the location where the borehole has penetrated the repository. The number of waste packages affected (i.e., the amount of inventory that becomes available) by the human intrusion activity is sampled between one and five (Section 3.1.2.9 for more detailed descriptions). ^{238}U is the dominant radionuclide in term of the mean release rate for the entire analysis time period. The dissolved ^{238}U concentration in the near-field water is limited by the solubility for the entire analysis time period. ^{239}Pu is the second dominant radionuclide for up to about 8×10^4 yr, then ^{93}Nb, ^{235}U, ^{237}Np, ^{135}Cs and ^{236}U become important by about the same degree. ^{93}Nb is a stable isotope and does not have dose consequence.

Figure 3.1-14 shows the mean mass release rate from the far-field overlying aquifer at 5 km from the boundary of repository footprint. For most radionuclides, the far-field mean release rates are substantially lower than the mean repository release rates due mainly to transport retardation by sorption on the aquifer materials and dilution in the aquifer. ^{238}U shows the highest mean release rate for the entire analysis time period, except the very early time period for up to about 1,400 yr, for which the highest mean release rate is by ^{36}Cl.

The calculated mean annual doses by individual radionuclides at the hypothetical accessible environment are shown in Figure 3.1-15. Although the far-field mean mass release rate is dominated by ^{238}U, other radionuclides dominate in terms of mean annual dose at different times: ^{14}C is the dominant mean annual dose contributor for about first 3×10^3 yr; ^{237}Np is the dominant mean annual dose contributor from about 3×10^3 yr to about 3.5×10^4 yr and again from about 2×10^5 yr to the end of analysis (1,000,000 yr); and ^{239}Pu is the dominant mean dose contributor from about 3.5×10^4 yr to about 2×10^5 yr This is the result mainly of much higher specific activity of the radionuclides (^{14}C: 4.47 Ci/yr, ^{239}Pu: 0.06 Ci/yr, ^{242}Pu: 0.004 Ci/yr, and ^{237}Np: 0.0007 Ci/yr) than ^{238}U (3.4×10^{-7} Ci/yr).

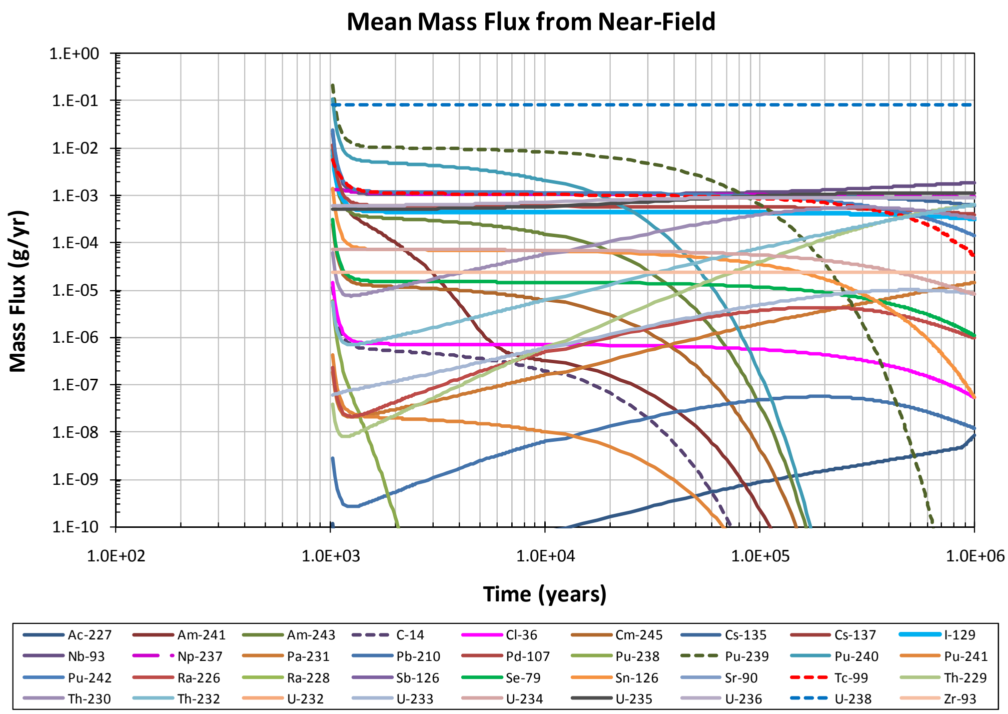


Figure 3.1-13. Model Results for Waste Inventory Case 1 of the Human Intrusion Scenario: Mean Release Rate from Repository

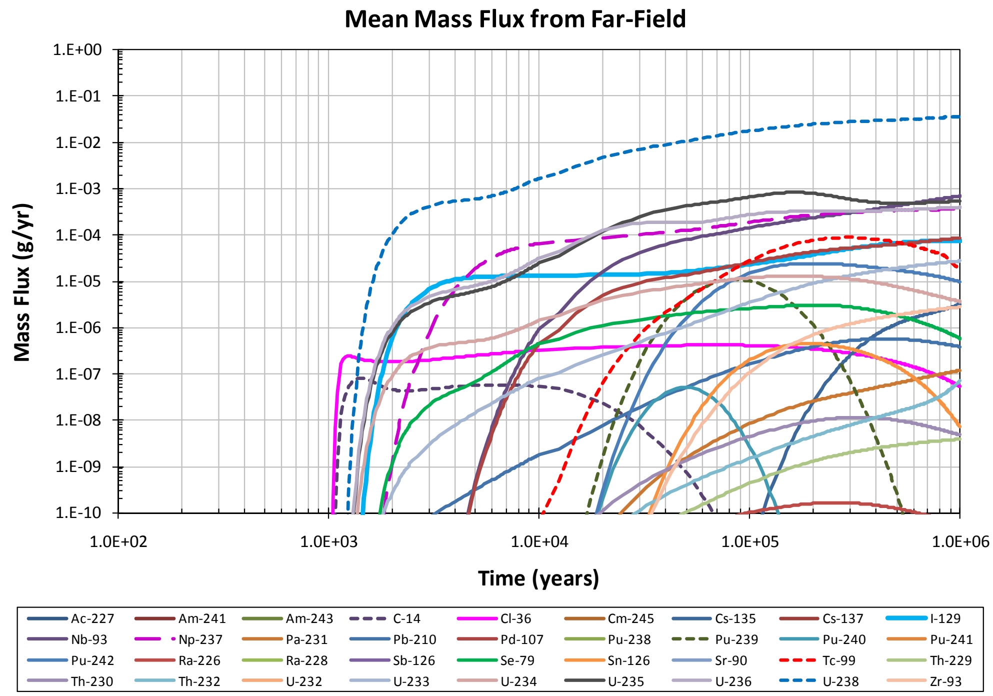


Figure 3.1-14. Model Results for Waste Inventory Case 1 of the Human Intrusion Scenario: Mean release Rate from the Far-Field Overlying Aquifer at 5 km from the Boundary of Repository Footprint

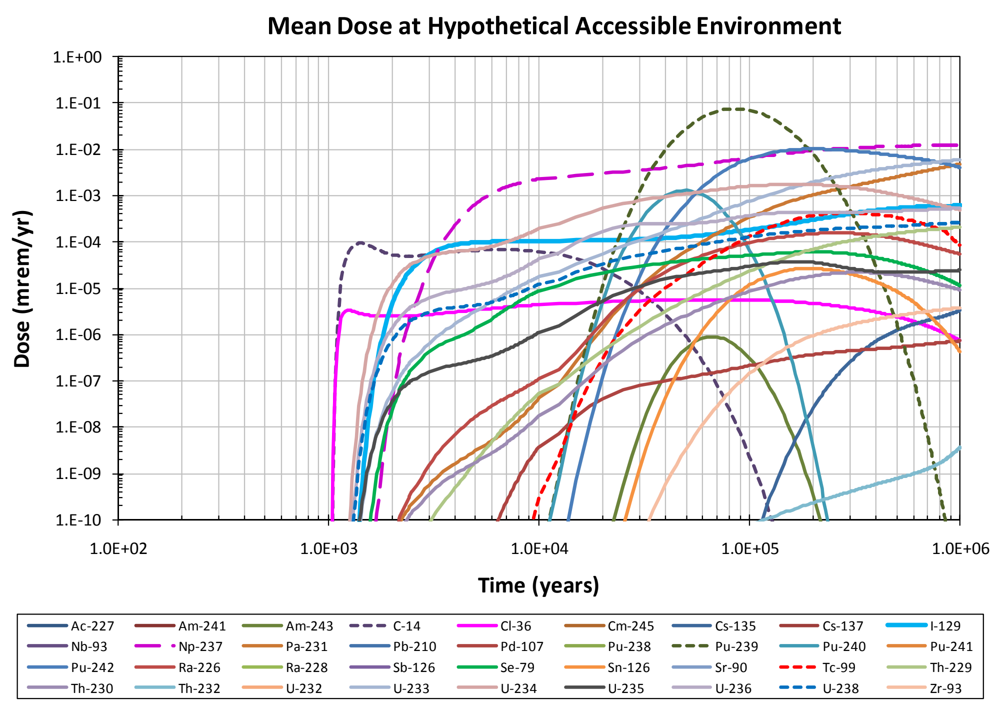


Figure 3.1-15. Model Results for Waste Inventory Case 1 of the Human Intrusion Scenario: Mean Annual Dose at the Hypothetical Accessible Environment at 5 km from the Boundary of Repository Footprint

3.1.4.2.2 Waste Inventory Case 2

Figure 3.1-16 shows the mean mass release rate from the repository through a borehole that has penetrated the repository at 1,000 yr after repository closure. The release rate is at the location where the borehole has penetrated the repository. Unlike Waste Inventory Case 1, ^{232}Th has the highest mean release rate until about 1.1×10^5 yr, thereafter ^{238}U becomes dominant for the mean mass release rate and ^{232}Th remains as the second dominant radionuclide. The high mean release rate of ^{232}Th is the outcome of the following factors: (1) high ^{232}Th inventory in the DHLW (3.5×10^4 g per waste package); (2) higher degradation rate of the glass waste form for the DHLW (mean fractional degradation rate of 4.9×10^{-4} per yr) than the UNF (mean fractional degradation rate of 1.5×10^{-7} per yr); and (3) higher solubility for thorium (mean solubility of 1,080 mg/L) than uranium (0.03 mg/L) in the near-field brine. As for Waste Inventory Case 1, dissolved ^{238}U concentration in the near-field water is limited by the solubility for the entire analysis time period.

The model results for the mean mass release rate from the far-field overlying aquifer at 5 km from the boundary of repository footprint are shown in Figure 3.1-17. The far-field mean release rates are substantially lower than the mean repository release rates because of transport retardation by sorption and dilution in the aquifer. ^{238}U has the highest mean release rate for the entire analysis time period except the first 500 yr after the borehole penetration during which ^{14}C is dominant. Although ^{232}Th has the highest mean repository release rate until about 1.1×10^5 yr and the second highest mean release rate thereafter, its far-field mean release rate is very low except during the very late time period of the analysis (after about 8×10^5 yr). This is the result of strong sorption of thorium on the aquifer materials (Table 3.1-9). The ^{235}U releases are also important for the entire analysis time period, with its mean release rate being comparable to that of ^{238}U until up to about 1×10^4 yr. It is interesting to note that the ^{79}Se mean release rate is comparable to the ^{235}U release rate until about 2.5×10^4 yr before it begins to decrease significantly. The early high mean release rates for ^{79}Se are not seen for Waste Inventory Case 1, and this is caused by the higher ^{79}Se inventory in the DHLW (109 g ^{79}Se per DHLW WP versus 32 g ^{79}Se per UNF waste package, see Tables 3.1-1 and 3.1-2) and the higher degradation rate of the glass waste form for the DHLW. ^{237}Np and ^{99}Tc are also important contributors to the long-term mean release rate from the far field.

Figure 3.1-18 shows mean doses by individual radionuclides at the hypothetical accessible environment located 5 km from the boundary of repository footprint. Similar to the Waste Inventory Case 1, although ^{238}U is the dominant radionuclide for the far-field mass release rate for the entire analysis time period, other radionuclides dominate in terms of mean annual dose at different time periods: ^{14}C is the dominant dose contributor until about 2.2×10^3 yr; ^{79}Se is the dominant dose contributor from about 2.2×10^3 yr to about 3.7×10^4 yr; ^{239}Pu is the dominant dose contributor from about 3.7×10^4 yr to about 1.7×10^5 yr; and ^{237}Np is the dominant dose contributor from about 1.7×10^5 yr to the end of analysis (1,000,000 yr). This is mainly the result of higher specific activity of the radionuclides (^{14}C: 4.47 Ci/yr, ^{239}Pu: 0.06 Ci/yr, ^{79}Se: 0.015 Ci/yr, and ^{237}Np: 0.0007 Ci/yr) than ^{238}U (3.4×10^{-7} Ci/yr).

The mean mass release rate and mean annual dose histories for the human intrusion scenario analysis are very different from those for the reference scenario analysis. Compared to the reference scenario results, the relative annual dose contributions by soluble, nonsorbing fission products, particularly ^{129}I, are much lower than by actinides including ^{239}Pu, ^{242}Pu and ^{237}Np. The lower relative mean annual dose contributions by the fission product radionuclides are due to their lower total inventory available for release (i.e., up to five affected waste packages), and the higher mean annual doses by the actinides are the outcome of the direct release of the radionuclides into an aquifer characterized by high water flow rates, thereby resulting in an early arrival of higher concentrations of the radionuclides at the biosphere drinking water well prior to their significant decay.

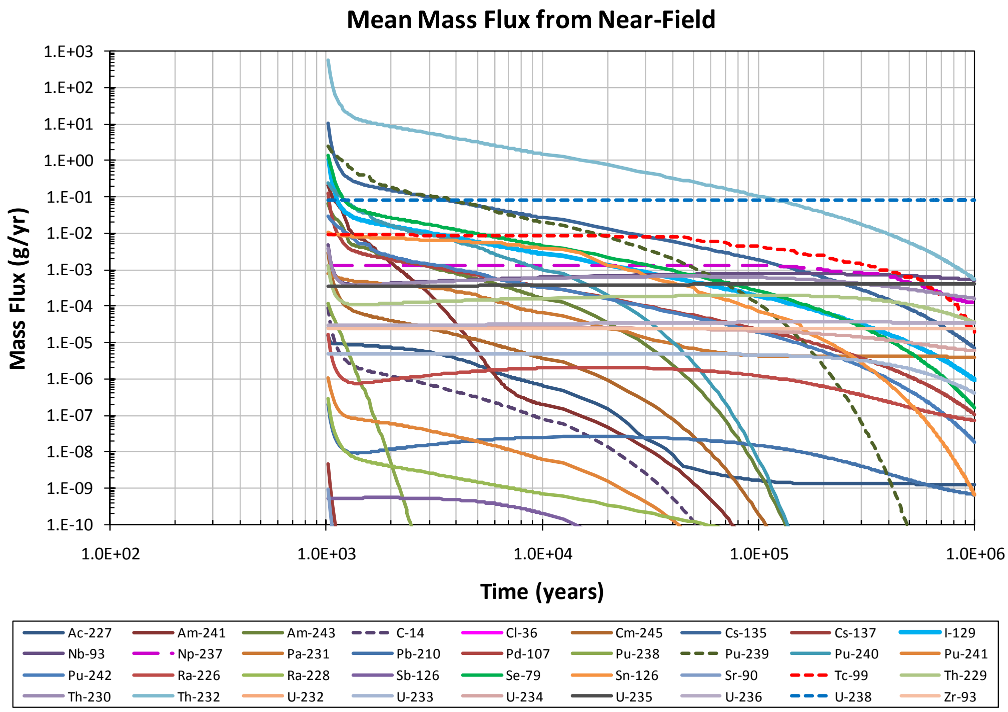


Figure 3.1-16. Model Results for Waste Inventory Case 2 of the Human Intrusion Scenario: Mean Release Rate from Repository

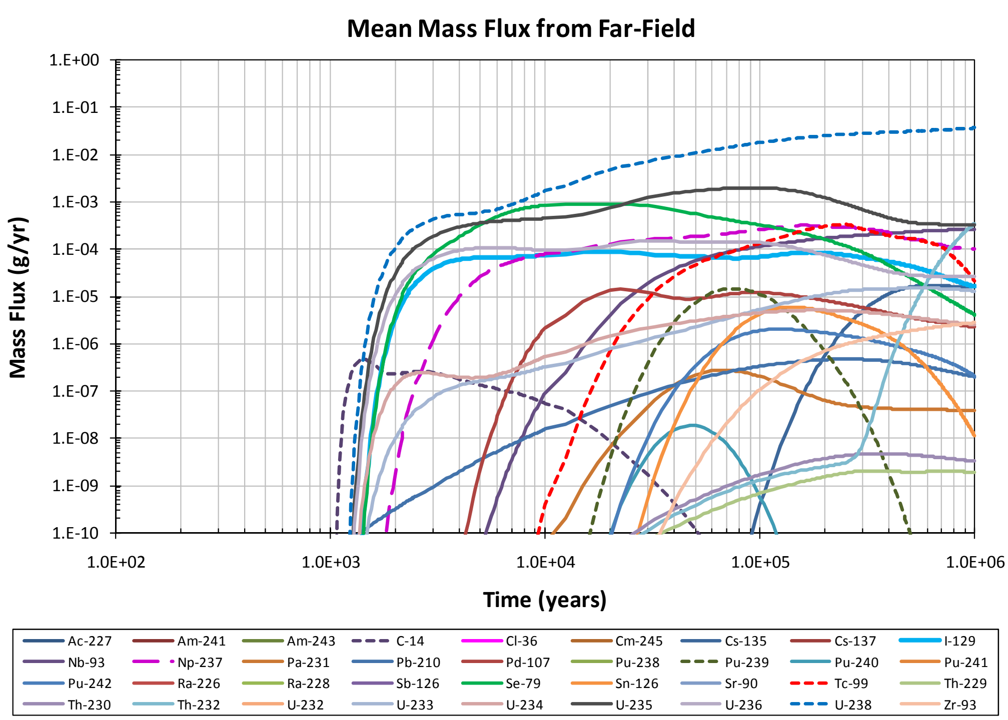


Figure 3.1-17. Model Results for Waste Inventory Case 2 of the Human Intrusion Scenario: Mean Release Rate from the Far-Field Overlying Aquifer at 5 km from the Boundary of Repository Footprint

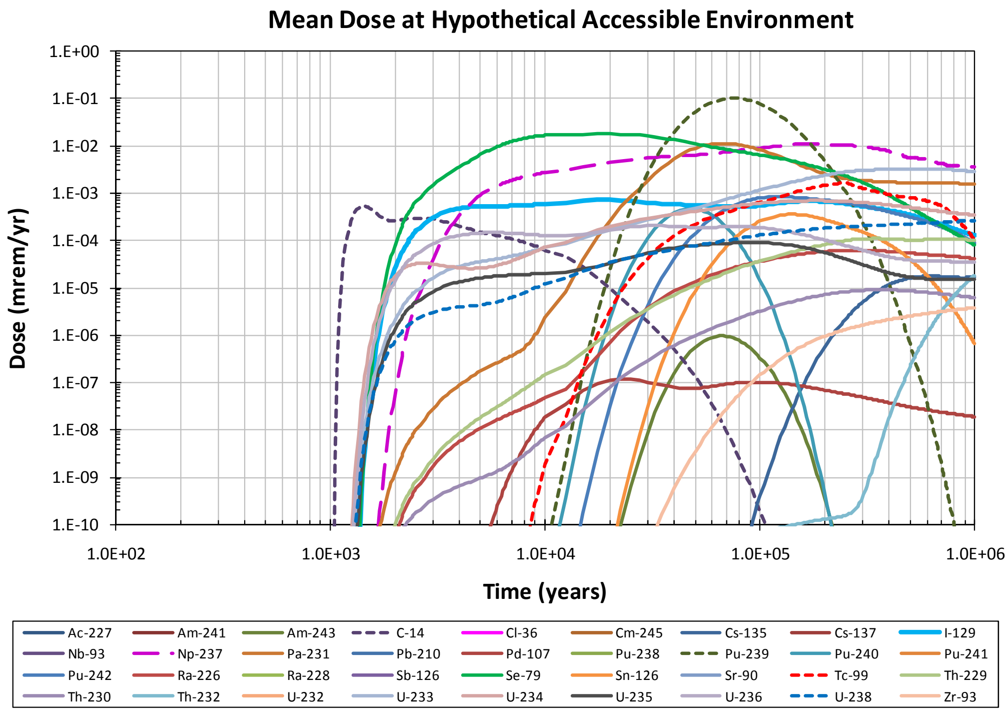


Figure 3.1-18. Model Results for Waste Inventory Case 2 of the Human Intrusion Scenario: Mean Annual Dose at the Hypothetical Accessible Environment at 5 km from the Boundary of Repository Footprint

3.1.5 Summary and Conclusions

Sections 3.1.1 through 3.1.4 document the current version of the salt GDS model and the preliminary results for the purpose of demonstrating capability. The immediate goal of the generic salt repository study is to develop the necessary modeling tools to evaluate and improve understanding on the repository system response and processes relevant to long-term disposal of UNF and HLW in salt. The current model represents a snap shot in the development process and will be further improved and refined as information from other UFD work packages matures. The vehicle for making these technical improvements will be the GPAM, which, because of its flexible architecture, will simulate repository performance for a variety of host rock and waste form options and at varying levels of sophistication that is appropriate to the applications at hand.

The current phase of the effort considered, where applicable, representative geologic settings and features adopted from literature data for salt repository sites. The conceptual model and scenario for radionuclide release and transport from a salt repository was developed utilizing literature data. The current salt GDS model consists of four major model components: source term, near field, far field, and biosphere. Specifically, the source-term and near-field model include the following components: (1) waste package configurations, (2) inventory for different waste types, (3) repository layout, (4) waste form degradation, (5) solubility of key radio-elements, (6) near-field volume, (7) repository waste inventory scenarios, and (8) repository radionuclide release scenarios.

The salt GDS model was developed in a probabilistic analysis framework. The example analysis for demonstration of model capability is for an isothermal condition at the ambient temperature for the near field.

The capability demonstration emphasizes key attributes of a salt repository that are potentially important to the long-term safe disposal of UNF and HLW. The analysis presents and discusses the results showing repository responses to different waste types (commercial UNF, existing DHLW, and hypothetical CHLW), and radionuclide release scenarios (undisturbed and human intrusion). In addition, knowledge gaps and paths forward for future R&D efforts to advance understanding of salt repository system performance for UNF and HLW disposal are provided.

For the reference (or nominal or undisturbed) scenario, the brine flow rates in the repository and underlying interbeds are very low, and transport of radionuclides in the transport pathways is dominated by diffusion and greatly retarded by sorption on the interbed filling materials. ^{129}I (nonsorbing and unlimited solubility with a very long half-life) is the dominant annual dose contributor at the hypothetical accessible environment, but the calculated mean annual dose is negligibly small that there is no meaningful consequence for the repository performance.

For the human intrusion (or disturbed) scenario analysis, the mean mass release rate and mean annual dose histories are very different from those for the reference scenario analysis. Compared to the reference scenario, the relative annual dose contributions by soluble, nonsorbing fission products, particularly ^{129}I, are much lower than by actinides including ^{239}Pu, ^{242}Pu and ^{237}Np. The lower relative mean annual dose contributions by the fission product radionuclides are due to their lower total inventory available for release (i.e., up to five affected waste packages), and the higher mean annual doses by the actinides are the outcome of the direct release of the radionuclides in the aquifer with high water flow rates, thereby resulting in an early arrival of higher concentrations of the radionuclides at the biosphere drinking water well prior to their significant decay.

The salt GDS model analysis has also identified the following future recommendations and/or knowledge gaps to improve and enhance the confidence of the future repository performance analysis.

- Repository thermal loading by UNF and HLW, and the effect on the engineered barrier and near-field performance.
- Closure and consolidation of salt rocks by creep deformation under the influence of thermal perturbation, and the effect on the engineered barrier and near-field performance.
- Brine migration and radionuclide transport under the influence of thermal perturbation in generic salt repository environment, and the effect on the engineered barrier and near-field performance and far-field performance.
- Near-field geochemistry and radionuclide mobility in generic salt repository environment (high ionic strength brines, elevated temperatures and chemically reducing condition).
- Degradation of engineer barrier components (waste package, waste canister, waste forms, etc.) in a generic salt repository environment (high ionic strength brines, elevated temperatures and chemically reducing condition).
- Waste stream types and inventory estimates, particularly for reprocessing high-level waste.

3.2 Granite GDS Model

The development of the granite GDS model and the preliminary model results are discussed in the subsections of Section 3.2. For consistency between generic disposal environments, many of the assumptions about model configurations developed for the salt GDS model (Section 3.1) were also applied to the granite GDS model.

3.2.1 Introduction

The granite GDS model is comprised of two major components: the near field and the far field. The granite GDS model adopts the near-field model template from the salt GDS model and incorporates an additional submodel of radionuclide diffusion through the bentonite buffer around waste packages in the near field. The far-field component of the granite GDS model is developed by incorporating the Finite Element Heat and Mass Transfer (FEHM) code (Zyvoloski et al. 1997; Zyvoloski 2007) into the GoldSim model (GoldSim Technology Group 2007).

The granite GDS model couples the near-field and the far-field components and a demonstration of capabilities is presented using PA simulations. The versions of codes used for this study are GoldSim (version 10.11) and FEHM (version 3.0). The model results were compared with simulation results (SKB 2010) from the SKB for confidence-building purposes. Monte Carlo simulations with the combined near- and far-field transport models were performed, and the model input parameter sensitivities were evaluated. A subset of radionuclides that could be potentially important to repository performance was identified and used as inventory. The analyses were conducted for two different repository radionuclide release scenarios. The capabilities of the tool presented here are being incorporated into the GPAM (Section 4) along with the capabilities of the models for the salt, clay, and deep borehole repository options. Technical improvements and capture of increased fundamental science describing the repository science associated with a generic granite host rock will in the future be developed within the GPAM framework. Once developed, GPAM will be used to provide guidance on the development of strategy for long-term disposal of UNF and HLW in a granite repository.

3.2.2 Model Description

The granite GDS model is comprised of two major components, the near field and the far field.

The near-field component encompasses waste form, the EBS, and the interface with the host rock. Note that some of the subject matter experts consider differing refinements in identifying the system model components (e.g. calling out the EBS as separate from the near field). These will be consistent in the GPAM framework. In the current granite GDS model, the near-field component includes the following:

- Repository layout and waste package configurations
- Radionuclide inventory and waste form degradation
- Solubility control and radionuclide release from waste panels
- Solubility control at the near-field and far-field interface

The current version of the model considered two radionuclide release scenarios:

- Disturbed - Human intrusion
- Undisturbed - Diffusion through bentonite buffer

The far-field component represents contaminant transport through the natural system from the near-field host rock to 100s or 1000s of meters; The FEHM code was coupled into the GoldSim system level model to represent the far-field component; it includes:

- Radionuclide decay and ingrowth
- Advection (residence time distribution (RTD)-based transport model, enable study of potentially very heterogeneous domains)
- Matrix diffusion (Generalized Dual Porosity Model, diffusive exchange between flowing porosity and surrounding rock matrix)
- Sorption
- Runtime input data altering program INPUTDAT

The granite GDS model is developed in GoldSim and couples the near-field and far-field components for PA simulations. Uncertainty in the expected behavior of a generic granite repository requires that the granite GDS model analyses be probabilistic in order to capture the likely range of potential outcomes. The granite GDS model evaluates likely future outcomes by conducting Monte Carlo multi-realization probabilistic simulations with LHS using probability distributions of uncertain parameters that may be important to a generic granite repository performance.

Two radionuclide release scenarios were considered using the granite GDS model: a disturbed scenario and an undisturbed scenario.

1. The disturbed scenario represents a situation that can be characterized using a fast pathway for radionuclide release to the far-field, and is modeled as a stylized human intrusion. In this implementation, the human intrusion scenario considers a single borehole penetration through a waste package at 1,000 yr after repository closure. The number of waste packages destroyed (one penetrated plus, if any, neighboring packages affected) is randomly sampled between one and five (uniform distribution). This represents the total amount of waste inventory that becomes available for release to an aquifer. This treatment of the human intrusion scenario does not consider a potential that waste could be directly brought up to the surface as a result of the drilling activities.
2. The undisturbed scenario represents a situation that can be characterized by potential radionuclide release resulting from a sequence of nominal processes that are expected to occur in a generic repository. Diffusion through bentonite buffer is considered as one potential undisturbed release process. Fractures in the surrounding granite may directly intersect some waste packages. Radionuclides released from these waste packages may be transported to the aquifer through fast fracture flows. The full inventory of breached waste packages that are intersected by a fracture provides the source term in this scenario. The number of breach waste packages is treated with uncertainty and is sampled between 0.1% to 1% of the total number of waste packages. The small fraction of breached waste packages is consistent with detailed analyses from the SKB program (SKB 2010).

Separate near-field models were developed and implemented for each of the two release scenarios. For both scenarios, the near-field model does not consider potential barrier performance of the waste packages, so the waste form starts to degrade and release radionuclides at time zero at the degradation rate used.

3.2.2.1 Overall Model Structure

The structure of the overall granite GDS model is shown in Figure 3.2-1. The near-field and far-field models are coupled through the near-far interface (*NF_interface*) component. This implementation of the model assumes that the repository is located in saturated granite with a chemically reducing environment below the water table. Consistent with the current reference design, the granite repository is assumed to have the same square footprint as the salt repository (Section 3.1.2.4) with 25-m spacing between emplacement tunnels and 6 m between waste packages. The granite GDS model also includes the same three waste types—commercial UNF, DHLW, and CHLW—and the same 36 radionuclides as the salt GDS model (Section 3.1.2.2). The granite GDS model assumes the same hypothetical biosphere as the salt GDS model (Section 3.1.2.8), located 5 km from the repository edge. The granite GDS model analysis runs 100 Monte-Carlo realizations for a time period of 1,000,000 yr.

The near-field model shown in Figure 3.2-2a includes the following major components:

- *Waste_form_degradation*—Calculate radionuclide release rates from waste degradation based on the assigned value of annual fraction waste form degradation rate.
- *WF_RN_release*—Calculate the radionuclide release rate to the near field as a function of waste form degradation, radionuclide solubility, and available water volume in the near field.
- *Repository_config & In_Package_volume*—Calculate the near-field void volume (i.e., the near-field water volume) of the granite GDS.

The far-field model shown in Figure 3.2-2b includes the far-field reactive transport model FEHM, which is implemented in GoldSim as a DLL and is discussed in Section 3.2.2.6. The *NF_interface* component shown in Figure 3.2-1 calculates the total radionuclide flux from the near field to the far field.

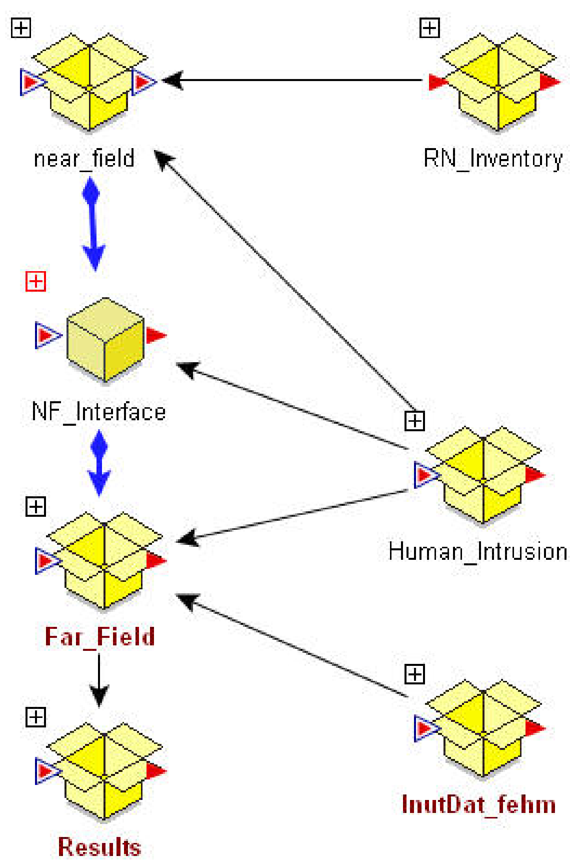
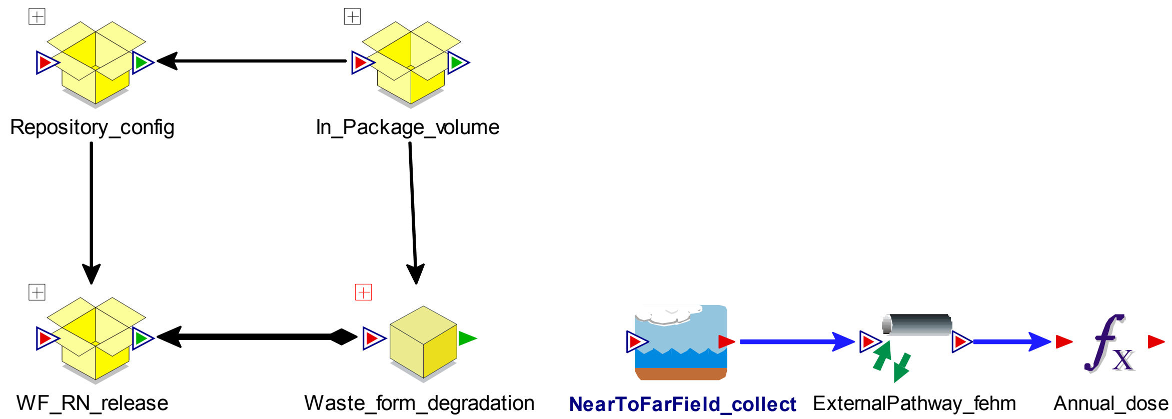


Figure 3.2-1. Overview of Structure of Granite GDS Model



(a) (b)

Figure 3.2-2. Granite GDS (a) Near-Field and (b) Far-Field Model Component Structure

3.2.2.2 Waste Form

3.2.2.2.1 Waste Inventory

The waste inventory for the granite GDS model is the same as for the salt GDS model (Section 3.1.2.2), based on a once-through fuel cycle waste inventory analysis (Carter and Luptak 2010). The three different types of waste—commercial UNF, DHLW, and CHLW—are summarized below. Further details are provided in Section 3.1.2.2.

Commercial UNF Inventory—A total of 140,000 MTU UNF is estimated to be discharged from reactors (Carter and Luptak 2010). For the granite GDS near-field model, this total commercial UNF inventory is represented by an equivalent inventory of 321,540 PWR assemblies. For the near-field model a single waste package is assumed to contain 10 PWR assemblies, for a total of 32,154 waste packages containing commercial UNF. The radionuclide inventory for commercial UNF is shown in Table 3.1-1.

DHLW Inventory—All existing DHLW is assumed to be immobilized in borosilicate glass logs. For the granite GDS near-field model, the DHLW is assumed to be contained 25,016 canisters (Carter and Luptak 2010). Each waste package is assumed to contain 5 DHLW canisters, for a total of 5,003 waste packages containing DHLW. The radionuclide inventory for DHLW is shown in Table 3.1-2.

CHLW Inventory—CHLW is assumed to be immobilized in the same borosilicate glass logs as DHLW, but with greater concentrations of fission products than the DHLW. The total radionuclide mass of CHLW is estimated to be 1,426 MT contained in a total of 20,276 canisters. The granite GDS near-field model assumes that each waste package contains five CHLW canisters, for a total of 4,055 waste packages containing CHLW. The radionuclide inventory for CHLW is shown in Table 3.1-3.

3.2.2.2.2 Waste Form Degradation

Waste form degradation for the granite GDS model is treated the same as for the salt GDS model (Section 3.1.2.5). For commercial UNF, the waste form is the UNF matrix, which is predominantly UO_2. For the DHLW and CHLW, the waste form is borosilicate glass. For both waste form types, the waste form degradation in the granite GDS near field is modeled with an annual fractional degradation rate (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates consistent with a generic granite host rock environment. The granite GDS near field is expected and assumed to be in water-saturated and chemically reducing conditions with varying degrees of redox conditions of groundwater in contact with the waste form. The chemically reducing conditions for the granite GDS are assumed to be same conditions as for the salt GDS. Therefore the same probabilistic degradation rate models for the UNF matrix and for the borosilicate glass were used (Section 3.1.2.5). As more information becomes available these may diverge in future analyses.

3.2.2.3 Waste Package

3.2.2.3.1 Waste Package Configurations

The waste package configuration for the granite GDS near-field model is the same as was assumed for the salt GDS model (Section 3.1.2.3), based on the waste cask design for SNF of the German salt disposal program (Janberg and Spilker 1998). The outer diameter of a waste package with bentonite buffer (0.36-m thickness) is 1.56 m, and the outer length is 5.5 m. Each waste package is assumed to hold 10 PWR commercial UNF assemblies, 5 DHLW canisters, or 5 CHLW canisters. Note that current thermal analyses suggest this will be too hot and that the model will need to be revised. The granite GDS analysis does not consider performance of waste package. Future conceptualizations are expected to take into account difference in waste package designs (and barrier potential) that might take advantage of the differing environments among salt, granite, and clay.

3.2.2.3.2 Reference Repository Layout

The reference repository layout for the granite GDS model is assumed to be the same square footprint as used in the salt GDS model (Section 3.1.2.4). The square repository footprint can be calculated from Equation 3.1-1 based on the number of waste packages, the length of waste package (5.5 m), the spacing between waste packages (6 m), and the spacing between emplacement tunnels (25 m). As for the salt GDS model, the waste package spacing and emplacement tunnel spacing were taken from the SKB repository design (Claesson and Probert 1996, SKB 2006).

3.2.2.3.3 Source-Term Water Volume

As described in Section 3.1.2.5, waste form degradation is assumed to release radionuclides into a large uniformly mixed container representative of the source-term water volume. The dissolved concentrations of radionuclides in the source-term mixing cell are then calculated based on the mass of the degraded radionuclides, the source-term water volume, and the radionuclide solubility. In the granite GDS model, the source-term bulk volume includes all of the degraded waste package materials (e.g., waste form, waste package internal materials, waste package, and bentonite buffer). This is a reasonable assumption for the granite GDS scoping analysis, considering that waste package performance is not taken into account and that the entire waste inventory becomes available from the beginning of analysis for interactions with the near-field environment releasing radionuclides into the near field. Note that this is a smaller source-term volume than is used in the salt GDS model, which assumes that the entire near field is included in the source-term volume (Sections 3.1.2.5 and 3.1.2.6).

3.2.2.4 Engineered Barrier System (EBS)

Bentonites have been proposed as buffer material for geological disposal of radioactive waste. In a water-saturated environment, the fluid in the bentonite buffer is almost static because of the very low permeability in the medium, and the advective transport through it is negligible (SKB 2010). The only significant transport process in the near field is the diffusion of radionuclides through the bentonite buffer coupled with radionuclide sorption to bentonite material. The granite GDS near-field model does not consider the potential performance benefits of waste packages; that is, waste forms start to degrade at time zero. This is a conservative assumption. The granite GDS near-field model includes a 0.36-m-thick bentonite buffer outside the waste package; the remaining space is filled with granite rock. The radionuclides are released through diffusion out of the bentonite buffer and into the intersected fracture.

The bentonite buffer properties, diffusivities, and sorption coefficients that affect the transport of key radionuclides are listed in Table 3.2-1.

3.2.2.5 Near Field

The near field represents physical domains and flow paths that control waste form dissolution, release of radionuclides, and radionuclide transport prior to radionuclides reaching the far field. Because the near-field thermal evolution information is not available, the implementation assumes an isothermal near field at an ambient temperature of 25°C. The current implementation of the granite GDS near-field model does not include waste package barrier performance or an EDZ. The near-field host rock is represented by granite bed rock with porosity range from 0.0005 to 0.01. Near-field model parameters are listed in Table 3.2-2.

Radionuclide solubility is an important parameter that controls dissolved concentrations of mobilized radionuclides in groundwater. Radionuclide solubility is affected at varying degrees by various geochemical conditions, including redox condition of contacting water, temperature, pH, and presence and concentration of other dissolved species. Because solubility analysis for representative groundwater for a generic granite repository site was not available, the granite GDS analysis considered the same two redox conditions for groundwater that were used in the salt GDS model (Section 3.1.2.6): (1) chemically reducing conditions based on a concentrated brine, and (2) less reducing or slightly oxidizing conditions based on a dilute brine. Because of expected thermal effects and the resulting concentration of the near-field groundwater in a granite GDS, the reducing-condition, concentrated brine is assumed to represent the groundwater in the granite GDS near field, and the less reducing or slightly oxidizing dilute brine is assumed to represent the groundwater in the granite GDS far field. The near-field water may experience elevated temperature conditions from the thermal perturbations caused by the decay heat of emplaced waste, but the current granite GDS model assumes the site ambient temperature (25°C) because the near-field thermal evolution information is not currently available and the thermal transients will be short lived with respect to the time frames involved and restricted spatially. Thermal aspects will be considered in the future as associated necessary information becomes available from other UFD work packages. The resulting elemental solubilities of key radionuclides used in the granite GDS analysis are given in Tables 3.2-3 and 3.2-4. The granite GDS elemental solubility values for U, Pu, Am, Np, Th, and Sn, derived from Wang and Lee (2010), are the same as for the salt GDS model. However, the elemental solubilities for Ac, C, Cl, Cm, Cs, I, Nb, Pa, Pd, Ra, Sb, Se, Sr, and Zr are all assumed to be unlimited in the granite GDS model. The current information is adequate from demonstrating capability and the solubility behavior in the granite GDS model will be replaced with behavior that is more representative of a granite environment as information becomes available.

3.2.2.6 Far Field

3.2.2.6.1 Reactive Transport Model – FEHM

The FEHM code (Zyvoloski et al. 1997; Zyvoloski 2007) is coupled to the GoldSim model as a DLL in order to represent processes that occur in the far-field component of the granite GDS model. This approach enables the full capabilities of FEHM to be employed in the calculation. In some instances, a process model of the natural system will be developed with a full 3D representation using a code like FEHM (e.g. the unsaturated and saturated zone components of the Yucca Mountain system). This capability is a significant improvement in the ability to integrate process level models in disposal system analyses.

Table 3.2-1. Bentonite Buffer Parameters Used in Granite GDS Model

Parameter	Stochastic Parameter Type	Base Case Value	Distribution Parameters
Density (kg/m^3)	Constant	2780	N/A
Porosity	Constant	0.18	N/A
Tortuosity	Constant	0.13	N/A
Thickness (m)	Constant	0.36	N/A
Effective Diffusivity D_e (m^2/s), Ac	Uniform	$2.52x10^{-8}$	Range: $5.1x10^{-10}$ – $5.0x10^{-8}$
D_e (m^2/s), Am	Uniform	$2.52x10^{-8}$	Range: $5.1x10^{-10}$ – $5.0x10^{-8}$
D_e (m^2/s), C	Constant	$8.8x10^{-10}$	N/A
D_e (m^2/s), Cl	Uniform	$8.55x10^{-12}$	Range: $4.1x10^{-12}$ – $1.3x10^{-11}$
D_e (m^2/s), Cm	Uniform	$2.52x10^{-8}$	Range: $5.1x10^{-10}$ – $5.0x10^{-8}$
D_e (m^2/s), Cs	Uniform	$9.52x10^{-9}$	Range: $2.04x10^{-9}$ – $1.7x10^{-8}$
D_e (m^2/s), I	Uniform	$1.14x10^{-9}$	Range: $3.0x10^{-11}$ – $2.24x10^{-9}$
D_e (m^2/s), Np	Uniform	$8.76x10^{-9}$	Range: $5.13x10^{-10}$ – $1.7x10^{-8}$
D_e (m^2/s), Pa	Uniform	$8.76x10^{-9}$	Range: $5.13x10^{-10}$ – $1.7x10^{-8}$
D_e (m^2/s), Pu	Uniform	$1.44x10^{-8}$	Range:$2.55x10^{-10}$ – $2.86x10^{-8}$
D_e (m^2/s), Ra	Uniform	$2.59x10^{-9}$	Range: $8.53x10^{-11}$ – $5.1x10^{-9}$
D_e (m^2/s), Se	Uniform	$2.92x10^{-11}$	Range: $7.1x10^{-12}$ – $5.13x10^{-11}$
D_e (m^2/s), Sn	Uniform	$7.81x10^{-10}$	Range: $1.8x10^{-10}$ – $1.38x10^{-9}$
D_e (m^2/s), Sr	Uniform	$2.59x10^{-9}$	Range: $8.53x10^{-11}$ – $5.1x10^{-9}$
D_e (m^2/s), Tc	Uniform	$9.35x10^{-8}$	Range: $8.5x10^{-8}$ – $1.02x10^{-7}$
D_e (m^2/s), Th	Uniform	$2.0x10^{-8}$	Range: $1.07x10^{-10}$ – $4.0x10^{-8}$
D_e (m^2/s), U	Uniform	$9.27x10^{-9}$	Range: $1.53x10^{-9}$ – $1.7x10^{-8}$
D_e (m^2/s), Nb	Constant	$8.97x10^{-11}$	N/A
D_e (m^2/s), Pb	Constant	$8.97x10^{-11}$	N/A
D_e (m^2/s), Pd	Constant	$8.97x10^{-11}$	N/A
D_e (m^2/s), Sb	Constant	$8.97x10^{-11}$	N/A
D_e (m^2/s), Zr	Constant	$8.97x10^{-11}$	N/A
Sorption Coefficient K_d (cc/g), Ac	Uniform	14850	Range: 300 – 29400
K_d (cc/g), Am	Uniform	14850	Range: 300 – 29400

Table 3.2-1. Bentonite Buffer Parameters Used in Granite GDS Model (continued)

Parameter	Stochastic Parameter Type	Base Case Value	Distribution Parameters
K_d (cc/g), C	Constant	5	N/A
K_d (cc/g), Cm	Uniform	14850	Range: 300 – 29400
K_d (cc/g), Cs	Uniform	560	Range: 120 – 1000
K_d (cc/g), I	Uniform	6.5	Range: 0 – 13
K_d (cc/g), Np	Uniform	515	Range: 30 – 1000
K_d (cc/g), Pa	Uniform	515	Range: 30 – 1000
K_d (cc/g), Pu	Uniform	8475	Range: 150 – 16800
K_d (cc/g), Ra	Uniform	1525	Range: 50 – 3000
K_d (cc/g), Se	Uniform	17	Range: 4 – 30
K_d (cc/g), Sn	Uniform	485.5	Range: 112 – 859
K_d (cc/g), Sr	Uniform	1525	Range: 50 – 3000
K_d (cc/g), Tc	Uniform	55000	Range: 50000 – 60000
K_d (cc/g), Th	Uniform	11782	Range: 63 – 23500
K_d (cc/g), U	Uniform	545	Range: 90 – 1000
K_d (cc/g), Cl	Constant	0	N/A
K_d (cc/g), Nb	Constant	0	N/A
K_d (cc/g), Pb	Constant	0	N/A
K_d (cc/g), Pd	Constant	0	N/A
K_d (cc/g), Sb	Constant	0	N/A
K_d (cc/g), Zr	Constant	0	N/A

Source: SKB 2010, Hansen et al. 2010; Itälä 2009; Montes-H et al. 2005; Pusch and Svemar 1993.

NOTE: For the species Nb, Pb, Pd, Sb, Zr and Cl, diffusion and/or sorption parameters were not readily available, and because this run was performed as a generic version to investigate the feasibility of the modeling system, placeholder values for diffusion and a sorption coefficient of 0 were used for computational expediency.

Table 3.2-2. Near-Field Parameters for 36 Radionuclides

Parameter	Stochastic Parameter Type	Base Case Value	Distribution Parameters
UNF Matrix Degradation Rate (1/yr)	Log-triangular	1.528×10^{-7}	1×10^{-8}, 1×10^{-7}, 1×10^{-6}
DHLW and CHLW Degradation Rate (borosilicate glass) (1/yr)	Log-uniform	4.917×10^{-4}	3.4×10^{-6}, 3.4×10^{-3}
Porosity, Inside Waste Package	Uniform	0.4	Range: 0.3 – 0.5
Porosity, Bed Rock	Uniform	0.00525	Range: 0.0005 – 0.01
Porosity, Overlaying Aquifer	Uniform	0.1	Range: 0.05 – 0.15
Waste Package Temperature (°C)	Constant	25	N/A
Waste Package Size, Outer Diameter (m)	Constant	1.56	N/A
Waste Package Size, Outer Length (m)	Constant	5.517	N/A
Number of Waste Packages – Commercial UNF	Constant	32154	N/A
Number of Waste Packages - DHLW	Constant	5003	N/A
Number of Waste Packages - CHLW	Constant	4055	N/A
Number of Waste Packages Affected by a Single Drilling through Repository	Uniform	3	Range: 1 – 5
Percent of Waste Packages Affected by Canister Failure and Diffuse through Bentonite Buffer (%)	Uniform	0.55	Range: 0.1 – 1
Portion of DHLW Waste Packages Affected by Canister Failure and Diffuse through Bentonite Buffer	Uniform	0.5	Range: 0 – 1
Water flow Rate up a Single Borehole through Granite GDS - Human Intrusion Scenario (m^3/yr)	Uniform	2.55	Range: 0.1 – 5
Water Flow Rate to Fracture Intersecting Commercial UNF Waste Package - Undisturbed Scenario (m^3/yr/per canister)	Constant	0.45×10^{-3}	N/A
Water Flow Rate to fracture Intersecting DHLW/CHLW Waste Package - Undisturbed Scenario (m^3/yr/per canister)	Constant	0.14×10^{-3}	N/A

Source: Neretnieks 1982; also see Section 3.1.2 for inventory and some near-field parameter references.

Table 3.2-3. Elemental Solubility of Select Radionuclides in Near-Field Concentrated Groundwater at 25°C

Element	Distribution Type	Solubility (mol/L)
U	Triangular	4.89E-08 (min); 1.12E-07 (mode); 2.57E-07 (max)
Pu	Triangular	1.40E-06 (min); 4.62E-06 (mode); 1.53E-05 (max)
Am	Triangular	1.85E-07 (min); 5.85E-07 (mode); 1.85E-06 (max)
Np	Triangular	4.79E-10 (min); 1.51E-09 (mode); 4.79E-09 (max)
Th	Triangular	2.00E-03 (min); 4.00E-03 (mode); 7.97E-03 (max)
Tc	Log-triangular	4.56E-10 (min); 1.33E-08 (mode); 3.91E-07 (max)
Sn	Triangular	9.87E-09 (min); 2.66E-08 (mode); 7.15E-08 (max)
C, Cl, Cs, I, Se, Sr	N/A	Unlimited solubility

NOTE: Elements Ac, Cm, Nb, Pa, Pd, Ra, Sb, Zr are known to be solubility limited, but are implemented as unlimited solubility in the near- and far-field model because their solubility calculations have not been completed.

In this implementation for demonstration, a generic approach to representing the far field captures the key hydrologic, and physical and chemical transport processes. A simple yet flexible far-field pathway model using FEHM has been developed for this purpose. The model consists of radionuclide decay and in-growth, advection, matrix diffusion, and sorption, all features that are implemented using FEHM's reactive transport modeling capability. The advection term is parameterized using a feature that enables the user to prescribe a distribution of advective travel times through a hydrologic pathway. This flexibility accounts for potentially very heterogeneous domains that may give rise to a broad distribution of advective transport times. Statistical parameters of the RTD, or an arbitrary distribution, are used and the model constructs a simplified pathway model that reproduces that distribution. This approach is called an RTD-based transport model. The groundwater velocity for generic granite GDS simulations is sampled through stochastic distribution with a mean value of 10 m/yr, the uncertainty about the mean is site specific and can vary plus or minus an order of magnitude (Joyce et al. 2010). In addition to the advective component, the model uses FEHM's Generalized Dual Porosity Model feature to account for diffusion

Table 3.2-4. Elemental Solubility of Select Radionuclides for Far-Field Dilute Groundwater at 25°C

Element	Distribution Type	Solubility (mol/L)
U	Triangular	9.16E-05 (min); 2.64E-04 (mode); 7.62E-04 (max)
Pu	Triangular	7.80E-07 (min); 2.58E-06 (mode); 8.55E-06 (max)
Am	Triangular	3.34E-07 (min); 1.06E-06 (mode); 3.34E-06 (max)
Np	Log-triangular	1.11E-06 (min); 1.11E-05 (mode); 1.11E-04 (max)
Th	Triangular	8.84E-06 (min); 1.76E-05 (mode); 3.52E-05 (max)
Sn	Triangular	1.78E-08 (min); 4.80E-08 (mode); 1.29E-07 (max)
C, Cl, Cs, I, Se, Sr, Tc	N/A	Unlimited solubility

NOTE: Elements Ac, Cm, Nb, Pa, Pd, Ra, Sb, Zr are known to be solubility limited, but are implemented as unlimited solubility in the near- and far-field model because their solubility calculations have not been completed.

between the flowing porosity and the surrounding rock matrix. Because the model is established using a numerical modeling approach in FEHM, the other relevant transport processes that are included in FEHM are also made available for inclusion. In this study, diffusion, radioactive decay and tracking of decay chains, and sorption (with an equilibrium "Kd approach") are used to generate the results that follow. An extensive theory was developed to implement this RTD-based model, the details of which are provided in Chu et al. (2008, Appendix B.1). Table 3.2-5 lists the far-field hydrologic parameters for 36 species. Parameters for representative radionuclides are summarized in Table 3.2-6.

3.2.2.6.2 FEHM Coupled with GoldSim

The FEHM code was modified to facilitate the coupling with GoldSim for probabilistic simulations for granite GDS studies. In the coupled model, GoldSim controls the overall time steps of the model run, and radionuclide mass is transferred to and from FEHM at each time step. This capability was implemented by using GoldSim Contaminant Transport Module External pathway, which calls FEHM as a DLL. At each time step, GoldSim passes a string of variables into each FEHM simulation to initialize the coupled simulation. These variables include: time, the number of species that FEHM will be simulating, and the amount of mass entering the groundwater pathway.

Table 3.2-5. Far-Field Hydrologic Parameters for 36 Radionuclide Species

Parameter	Stochastic Parameter Type	Base Case Value	Distribution Parameters
Flow Parameters			
Mean of Ln Travel Time Distribution, μ_{ln}	Normal distribution for μ_{ln}	23.482 (ln(s))	23.482, 0.8
Std. Dev. of Ln Travel Time Distribution, σ_{ln}	Normal distribution for $\bar{\sigma}_{ln} = \sigma_{ln} / \mu_{ln}$	0.026487	0.026487, 7.946×10^{-3}
Geometric Parameters			
Aperture (m)	Uniform	0.000255	Range: 1.0×10^{-5} – 5.0×10^{-4}
Fracture Spacing (m)	Constant	25	N/A
Transport Parameters			
Diffusive Tortuosity τ_D, all species	Normal distribution for $\tau_D = D / D_{free}$	0.0144	0.0144, 4.176×10^{-3}
Free-Water diffusion coefficient D_{free} (m^2/s), Am	Constant	9.49×10^{-10}	N/A
D_{free} (m^2/s), C	Constant	1.18×10^{-9}	N/A
D_{free} (m^2/s), Pa	Constant	6.04×10^{-10}	N/A
D_{free} (m^2/s), Ra	Constant	8.89×10^{-10}	N/A
D_{free} (m^2/s), Th	Constant	5.97×10^{-10}	N/A
D_{free} (m^2/s), Sn	Constant	1.55×10^{-9}	N/A
D_{free} (m^2/s), Cl	Constant	2.03×10^{-9}	N/A
D_{free} (m^2/s), Cs	Constant	2.06×10^{-9}	N/A
D_{free} (m^2/s), I	Constant	2.05×10^{-9}	N/A
D_{free} (m^2/s), Np	Constant	6.18×10^{-10}	N/A
D_{free} (m^2/s), Se	Constant	1.04×10^{-9}	N/A
D_{free} (m^2/s), Sr	Constant	7.91×10^{-10}	N/A
D_{free} (m^2/s), Tc	Constant	1.95×10^{-9}	N/A
D_{free} (m^2/s), U	Constant	6.64×10^{-10}	N/A
Matrix Diffusion Coefficient (pore diffusivity) D (m^2/s), Cl	Truncated normal distribution	1.37×10^{-10}	Range:3.75×10^{-11} – 3.21×10^{-10}, 1.37×10^{-10}, 1.08×10^{-10}

Table 3.2-5. Far-Field Hydrologic Parameters for 36 Radionuclide Species (continued)

Parameter	Stochastic Parameter Type	Base Case Value	Distribution Parameters
D (m^2/s), Cs	Truncated normal distribution	2.11×10^{-10}	Range:1.03×10^{-10} – 3.75×10^{-10}, 2.11×10^{-10}, 1.05×10^{-10}
D (m^2/s), I	Truncated normal distribution	1.57×10^{-10}	Range:7.96×10^{-11} – 3.38×10^{-10}, 1.57×10^{-10}, 6.02×10^{-10}
D (m^2/s), Np	Truncated normal distribution	6.99×10^{-11}	Range:2.8×10^{-11} – 1.1×10^{-10}, 6.99×10^{-11}, 2.75×10^{-11}
D (m^2/s), Pu	Truncated normal distribution	4.1×10^{-11}	Range:2.61×10^{-11} – 5.63×10^{-11}, 4.1×10^{-11}, 1.07×10^{-11}
D (m^2/s), Se	Truncated normal distribution	8.93×10^{-11}	Range:8.26×10^{-11} – 9.46×10^{-11}, 8.93×10^{-11}, 5.0×10^{-12}
D (m^2/s), Sr	Truncated normal distribution	6.65×10^{-11}	Range:2.86×10^{-11} – 4.0×10^{-10}, 6.65×10^{-11}, 9.66×10^{-11}
D (m^2/s), Tc	constant	4.2×10^{-12}	N/A
D (m^2/s), U	Truncated normal distribution	5.14×10^{-12}	Range:3.14×10^{-12} – 6.29×10^{-12}, 5.14×10^{-12}, 1.42×10^{-12}
D (m^2/s), Ac	Constant	5.0×10^{-11}	N/A
D (m^2/s), Pb	Constant	5.0×10^{-11}	N/A
D (m^2/s), Sb	Constant	5.0×10^{-11}	N/A
D (m^2/s), Zr	Constant	5.0×10^{-11}	N/A
D (m^2/s), Nb	Constant	5.0×10^{-11}	N/A
D (m^2/s), Pd	Constant	5.0×10^{-11}	N/A
D (m^2/s), Cm	Constant	5.0×10^{-11}	N/A
Matrix Sorption Coefficient K_d (cc/g), Ac	CDF	3000	(1000,0) (3000,0.5) (5000,1)
K_d (cc/g), Am	CDF	3000	(1000,0) (3000,0.5) (5000,1)
K_d (cc/g), C	CDF	1	(0.5,0) (1,0.5) (2,1)
K_d (cc/g), Cl	Nonsorbing	0	0
K_d (cc/g), Cm	CDF	3000	(1000,0) (3000,0.5) (5000,1)
K_d (cc/g), Cs	CDF	500	(100,0) (500,0.5) (1000,1)
K_d (cc/g), I	Nonsorbing	0	N/A
K_d (cc/g), Nb	CDF	1000	(500,0) (1000,0.5) (3000,1)

Table 3.2-5. Far-Field Hydrologic Parameters for 36 Radionuclide Species (continued)

Parameter	Stochastic Parameter Type	Base Case Value	Distribution Parameters
K_d (cc/g), Np	CDF	5000	(1000,0) (5000,0.5)(10000,1)
K_d (cc/g), Pa	CDF	1000	(500,0) (1000,0.5) (5000,1)
K_d (cc/g), Pd	CDF	100	(10,0) (100,0.5) (500,1)
K_d (cc/g), Pu	CDF	5000	(1000,0) (5000,0.5)(10000,1)
K_d (cc/g), Ra	CDF	100	(50,0) (100,0.5) (500,1)
K_d (cc/g), Se	CDF	1	(0.5,0) (1,0.5) (5,1)
K_d (cc/g), Sn	CDF	1	(0,0) (1,0.5) (10,1)
K_d (cc/g), Sr	CDF	10	(5,0) (10,0.5) (50,1)
K_d (cc/g), Tc	CDF	1000	(300,0) (1000, 0.5) (3000,1)
K_d (cc/g), Th	CDF	5000	(1000,0) (5000,0.5)(10000,1)
K_d (cc/g), U	CDF	5000	(1000,0) (5000,0.5)(10000,1)
K_d (cc/g), Zr	CDF	1000	(500,0) (1000,0.5) (3000,1)
K_d (cc/g), Pb	Constant	0	N/A
K_d (cc/g), Sb	Constant	0	N/A

Source: Carbol and Engkvist 1997; JAEA n.d.; Chu et. al. 2008.

NOTE: For Ac, Pb, Sb, Zr, Nb, Pd and Cm, diffusion parameters were not readily available (sorption parameters are not readily available for Pb, Sb), and because the model analysis was performed for a generic repository to investigate the feasibility of the modeling system, placeholder values for diffusion and a sorption coefficient of 0 were used for expediency.

GoldSim initializes the simulation by passing the first time increment to FEHM. In the FEHM simulation, GoldSim passes the mass associated with each radionuclide arriving into the groundwater pathway during that time step. FEHM accepts the incoming mass and adds it to the ongoing calculation of transport through the RTD-based representation of pathways in the far field. The cumulative transport of each species, accounting for radioactive decay, is calculated. FEHM can be invoked in a way that enables multiple, smaller time steps to be taken within each GoldSim time step to ensure that the tracer transport solution converges to an accurate solution. At the end of each GoldSim time step, FEHM passes back into GoldSim any mass reaching the far-field boundary. Mass reaching the far-field boundary originates either from the initial source term or in-growth of daughter products formed during transport along the groundwater pathway.

The FEHM input data files contain inputs such as diffusion and sorption parameters that are to be generated from a stochastic distributions. To accomplish this in a flexible way, a separate DLL was developed and used to alter the data in the FEHM input files at the beginning of each realization. The DLL INPUTDAT is invoked by GoldSim initially, before GoldSim executes FEHM, to generate an input data file for each FEHM realization run. For each realization, the INPUTDAT program samples the input parameters from a stochastic distribution generated by GoldSim, and places them in the correct places in

Table 3.2-6. Parameters for Representative Radionuclides

Species ID	Atomic Weight (g/mol)	Half-Life (yr)	Solubility – Near Field (mg/L)	Solubility – Near- / Far-Field Interface (mg/L)	Far-Field Sorption Coefficient Kd (cc/g)	Specific Activity (Ci/g)	Dose Conversion Factor (Sv y^{-1} / Bq y^{-1})
Actinide Parent Species							
Np	237	2.14×10^{6}	5.36×10^{-4}	4.003	5000	0.00070487	1.33×10^{-11}
Pu	238 239 240 242	87.7 2.41×10^{4} 6.54×10^{3} 3.76×10^{5}	1.721	0.961	5000	17.127 0.062066 0.22776 0.0039289	2.76×10^{-11} 3.00×10^{-11} 3.00×10^{-11} 2.88×10^{-11}
Am	241 243	432 7.37×10^{3}	2.12×10^{-1}	3.83×10^{-1}	3000	3.4338 0.19962	2.40×10^{-11} 2.41×10^{-11}
U	232 233 234 235 236 238	68.9 1.59×10^{5} 2.45×10^{5} 7.04×10^{8} 2.34×10^{7} 4.46×10^{9}	3.315×10^{-2}	8.857×10^{1}	5000	22.365 0.0096498 0.0062357 2.1609×10^{-6} 6.4736×10^{-5} 3.3679×10^{-7}	6.7×10^{-11} 6.12×10^{-12} 5.88×10^{-12} 5.68×10^{-12} 5.64×10^{-12} 5.81×10^{-12}
Fission Products and Others							
Tc	99	2.13x105	3.165×10^{-3}	unlimited	1000	0.016953	7.68×10^{-14}
I	129	1.57x107	unlimited	unlimited	0	0.00017651	1.32×10^{-11}
Cs	135	2.3x106	unlimited	unlimited	500	0.0011514	2.40×10^{-13}
Se	79	3.27 x105	unlimited	unlimited	1	0.013839	3.48×10^{-13}
Cl	36	3.01 x105	unlimited	unlimited	0	0.032991	1.116×10^{-13}

Source: Carbol and Engkvist 1997; JAEA n.d.; Chu et al. 2008.

the input data template to create a new input data file for that FEHM realization. This development was done in a general way, such that any parameter in the FEHM input file can be generated stochastically and placed into the file at runtime.

3.2.2.7 Aquifer

The granite GDS model assumes a shallow bedrock aquifer near the surface; the current version of model treats the aquifer as part of the far field.

3.2.2.8 Biosphere

A hypothetical biosphere is assumed to be located 5 km from the repository edge. The IAEA BIOMASS ERB1B dose model is used to convert the output radionuclide concentrations in the ground water at the hypothetical drinking well location to an estimate of annual dose based on drinking well water consumption (IAEA 2003). The biosphere model and parameter values for the granite GDS biosphere are the same as for the salt GDS biosphere (Section 3.1.2.8).

3.2.3 Confidence Building and Demonstration of Capability

3.2.3.1 Confidence Building

This subsection discusses the confidence-building simulations performed for the granite GDS model. The results generated by the granite GDS model were compared with results (SKB 2010) from the SKB safety assessment SR-site for the deterministic isostatic collapse scenario. The scenario, a hypothetical scenario used to assess barrier function (SKB 2010), postulates a single waste package failure at 10,000 yr. The barrier function of the waste package is lost, but the bentonite buffer remains intact.

The SKB assessment modeled three transport paths:

- *Q1*—A fracture intersecting the deposition hole at the vertical position of the canister lid. This fracture is placed on the opposite side of the buffer to the canister defect, hence minimizing the transport distance and the diffusional transport resistance. Thermally induced spalling is assumed to have occurred in the wall of the deposition hole meaning that the transport resistance at the interface Q1 is decreased.
- *Q2*—An EDZ in the floor of the deposition tunnel. In the hydrogeological model, EDZ is treated as a thin conductive layer.
- *Q3*—A fracture intersecting the deposition tunnel. The distance to Q3 is obtained in the hydrogeological model by tracing advectively transported particles released in the deposition tunnel just above the deposition hole. Since the distance from the deposition hole to Q3 differs, the longitudinal dimensions of the modeled deposition tunnel are different for different deposition holes.

Table 3.2-7. SKB Canister Failure Simulation Parameters

Parameter	^{129}I	^{79}Se	^{14}C
Inventory (g/canister)	348.3	10.744	0.5166
Solubility (mg/L)	Unlimited	$5.293x10^{-4}$	Unlimited
Effective Diffusion Coefficient (m^2/s), Buffer	7.922×10^{-12}	7.922×10^{-12}	1.33×10^{-10}
Effective Diffusion Coefficient (m^2/s), Rock	6.338×10^{-15}	6.338×10^{-15}	1.996×10^{-14}
Sorption Coefficient (m^3/kg), Buffer	Nonsorbing	Nonsorbing	Nonsorbing
Sorption Coefficient (m^3/kg), Rock	Nonsorbing	Nonsorbing	Nonsorbing
Porosity, Buffer	0.18	0.18	0.45
Porosity, Rock	0.0018	0.0018	0.0018
Half-Life (yr)	1.57×10^{7}	3.27×10^{5}	5.71×10^{3}
Dose Conversion Factors (Sv/yr per Bq/yr)	6.46×10^{-10}	1.21×10^{-9}	5.44×10^{-12}

Source: SKB 2010.

Table 3.2-8. Hydrologic and Transport Parameters for Case with SKB Canister Failure at 10,000 yr

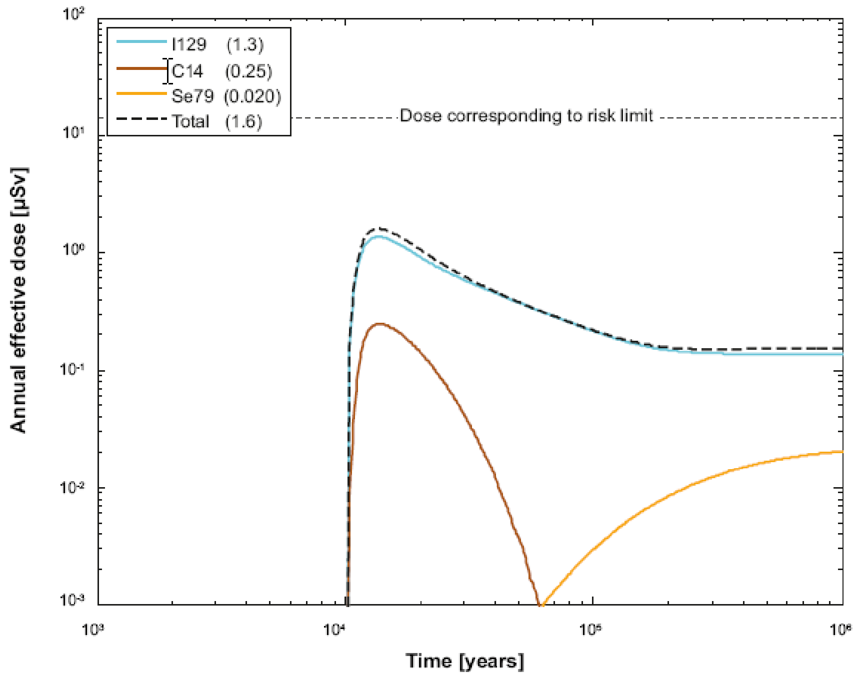
Parameter	Value
Far-Field Path Length (m)	500
Buffer Thickness (m)	0.35
Buffer Porosity	0.18
Buffer Density (kg/m3)	2780
Flow Rate for Q1 Release Path (m^3/yr)	4.2×10^{-6}
Rock Transport Resistance for Path Q1 (yr/m)	4.00×10^{6}
Rock Advective Travel Time for Path Q1 (yr)	1.8×10^{2}
Flow Rate for Q2 Release Path (m^3/yr)	9.3×10^{-5}
Rock Transport Resistance for Path Q2 (yr/m)	2.30×10^{6}
Rock Advective Travel Time for Path Q2 (yr)	1.6×10^{2}
Flow Rate for Q3 Release Path (m^3/yr)	1.2×10^{-4}
Rock Transport Resistance for Path Q3 (yr/m)	1.90×10^{6}
Rock Advective Travel Time for Path Q3 (yr)	1.5×10^{2}

Source: SKB 2010.

A deterministic calculation of the one canister failure at 10,000 yr was performed. Table 3.2-1 shows the input parameters for 3 species ^{129}I, ^{79}Se, and ^{14}C. Table 3.2-2 lists the hydrologic and transport parameters for this simulation.

The results from the SKB assessment one canister failure at 10,000 yr scenario are shown in Figure 3.2-3, and the results from the granite GDS model with similar radionuclides release scenario are shown in Figure 3.2-4. Note, for the granite GDS model simulation, it is assumed the inventories are not bound within matrix. The waste will be all available for release once the canister fails at 10,000 yr. This was not the case for the SKB simulation, which had some fraction of inventories bound within matrix and some fraction not bound.

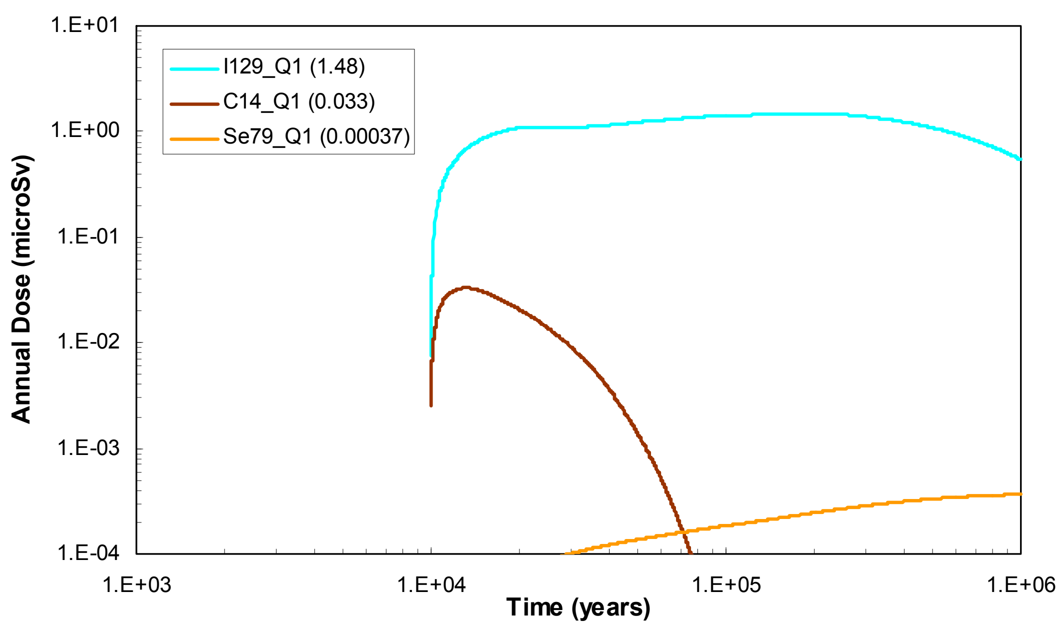
Overall, the patterns are very similar in terms of breakthrough time and peak in comparison with SKB results. For Q1 release path, granite GDS model (Figure 3.2-4) ^{129}I having highest peak dose of 1.48 μSv/yr (1.48×10^{-1} mrem/yr), ^{14}C peak annual dose of 0.033 μSv/yr (3.3×10^{-3} mrem/yr), and ^{79}Se peak annual dose of 0.00037 μSv/yr (3.7×10^{-5} mrem/yr). The difference in detailed release mechanisms for different radionuclide and model configuration may contribute to the lower selenium dose rate. The current version of the granite GDS model does not include waste package barrier performance or an EDZ, as was the case in the SKB model.



Source: SKB 2010.

NOTE: The legend is sorted by peak (in the 1,000,000-yr period) of the annual effective dose. The values in brackets are peak dose in units of µSv/yr.

Figure 3.2-3. SKB Far-Field Annual Effective Dose for a Deterministic Calculation of Case with One Canister Failure at 10,000 yr



NOTE: The values in brackets are peak dose in units of µSv/yr.

Figure 3.2-4. Granite GDS Model Far-Field Annual Dose for a Deterministic Calculation of Case with Canister Failure at 10,000 yr Assuming Waste Not Bound to Matrix (Q1 Release Path)

3.2.3.2 Demonstration of Capability

3.2.3.2.1 Disturbed and Undisturbed Scenarios

This subsection discusses the preliminary results of the granite GDS model analysis. The coupling between the near-field and the far-field model is handled as follows: the far-field model takes the total mass flux output from the near-field model as the input mass flux to carry out the far-field transport by FEHM. Parameters for representative radionuclides, bentonite buffer, near and far-field transport can be found in Section 3.2.2. Note that parameter ranges and distributions are selected just for a demonstration purpose of the granite GDS model analysis (Hansen et al. 2010; Itälä 2009; Montes-H et al. 2005; Pusch and Svemar 1993; Neretnieks 1982; Carbol and Engkvist 1997; JAEA n.d.).

As noted in Section 3.2.2, two independent radionuclide release scenarios are simulated with the granite GDS model:

1. *Disturbed Scenario (human intrusion)*—Assume a single borehole penetrates through the repository at 1,000 yr, thus creating a fast pathway for radionuclide transport to the aquifer. The flow rate up the borehole is sampled through a stochastic distribution with a mean value 2.55 m^3/yr. The number of waste packages affected (i.e., waste inventory affected) by a single borehole penetration is sampled between 1 and 5. It is assumed that only commercial UNF waste packages are affected by human intrusion. No DHLW inventory is affected. This assumption was chosen as a simplification and is consistent with the Human Intrusion Scenario Case 1 evaluated with the salt GDS model (Section 3.1.4.2).
2. *Undisturbed Scenario (diffusion through bentonite buffer)*—In this scenario radionuclides released from degrading waste form are transported away from the waste package by diffusion through the bentonite buffer; the advective transport through it is negligible (SKB 2010). Some waste packages directly intersect with fractures in the surrounding granite rock, and radionuclides released from these waste packages directly enter into the fractures for fast pathway transport. The flow rate upward in the intersected fractures is sampled with a mean value of 0.45×10^{-3} m^3/yr per waste package for commercial UNF and 0.14×10^{-3} m^3/yr per waste package for DHLW and CHLW. The upward flow rate can be influenced by the waste package geometry. Here different flow rates are sampled for different types of waste package to reflect this effect. For those waste packages releasing radionuclides to the fractures, the model assumes that a fraction (between 0.1% and 1%) of the considered inventory is available for the advective transport in the fractures, and the fraction is sampled uniformly between the bounds. Inventory considered for this scenario includes commercial UNF plus DHLW.

The radionuclide mass fluxes (converted to an annual dose) at the location of the hypothetical biosphere (5 km downstream from the repository boundary) were analyzed. The simulations were run for 1,000,000 yr with 100 Monte Carlo realizations for each scenario listed above.

The granite GDS model has the capability to simulate the same two waste inventory cases considered for the salt GDS model (Section 3.1.4.1): Waste Inventory Case 1, which comprises the commercial UNF and DHLW, and Waste Inventory Case 2 comprises the DHLW and CHLW. These two inventory cases are incorporated in the granite GDS near-field model with a simple module to switch from one case to the other. The granite GDS model results presented in this subsection all use Waste Inventory Case 1, which considers a total of 37,157 waste packages (32,154 commercial UNF waste packages plus 5,003 DHLW waste packages) within a square repository footprint with a side of 3,270 m. However, as noted above, for the human intrusion scenario, no DHLW is affected, so Human Intrusion Case 1 includes only commercial UNF waste packages.

Figure 3.2-5 shows the mean annual doses of individual radionuclides at the hypothetical biosphere location (5 km downstream from the repository boundary) for Human Intrusion Case 1, calculated from 100 realizations simulations. The ^{129}I mean annual dose (the highest dose brown color line in Figure 3.2-5) surpasses ^{241}Am, ^{243}Am, ^{239}Pu and ^{240}Pu after a few thousand years, and eventually becomes the dominant contributor toward the end of the 1,000,000-yr time period. The long half-life, high solubility, and weak sorption in the far field of ^{129}I contribute to its higher mean dose. ^{226}Ra shows as the second highest mean annual dose species.

Figure 3.2-6 shows mean annual doses of individual radionuclides at the hypothetical biosphere location for undisturbed scenario, release by diffusion through bentonite buffer. Compared with human intrusion scenario, the dose rates are much lower at early time. Again the ^{129}I mean annual dose (the highest dose brown color line in Figure 3.2-6) catches up after a few thousand years, eventually becomes the dominant contributor toward the end of the 1,000,000-yr time period.

3.2.3.2.2 Sensitivity Analysis

A benefit of probabilistic analysis of GDSs is that the relative importance of various uncertain processes can be examined through a statistical analysis of the Monte Carlo results. This analysis can guide future work planning to prioritize research needs, to reduce uncertainties in the model analysis or in other ways improve the model. Figures 3.2-7(a) and 7(b) illustrated this process.

The annual doses were analyzed using a sensitivity analysis tool (Saltelli and Tarantola 2002) provided as part of the GoldSim software. The importance analysis of the input variables to the results are statistical measures computed by analyzing multiple realizations of the model in which all of the stochastic variables are simultaneously sampled for each realization of a Monte Carlo simulation. The importance measure is a metric that varies between 0 and 1 representing the fraction of the result's variance that is explained by a given variable treated with uncertainty. This measure is useful in identifying nonlinear, nonmonotonic relationships between an input variable and the result (which conventional correlation coefficients may not reveal).

Important parameter uncertainties influencing the overall uncertainty in performance (as measured by the annual dose in this study) depends on the time frame of interest. Each relevant parameter was ranked in order of importance to the overall uncertainty with respect to the annual dose reached at 10^4, 10^5, and 10^6 yr. The importance measures shown in following figures are normalized for each time stage so that they can be compared among different time frame of interest.

Figure 3.2-7(a) shows the sensitivity analysis of input parameters with respect to the uncertainties of ^{129}I annual dose at different times for the Human Intrusion Case 1 release scenario using commercial UNF only. It shows that uncertainty in the mean travel time of water in the far-field (LnorMean), granite bedrock porosity (Porosity_bedrock) and the commercial UNF waste form degradation rate (UNF_WF_rate) have dominant influences on uncertainty in the ^{129}I annual dose at 10,000 yr. The LnorMean and bedrock porosity have decreasing influences with time. The UNF_WF_rate's influence increases near the end of simulation duration. This shows that at lower UNF fractional degradation rate for nonsorbing (in far field) radionuclides such as ^{129}I, the annual dose is controlled more by the uncertainties in the near field than by the uncertainty in the far-field transport as time increases.

Figure 3.2-7(b) shows sensitivity analysis of input parameters with respect to the uncertainties of ^{129}I annual dose at different times for the Undisturbed Case 1 release scenario using commercial UNF and DHLW. It shows that the granite bedrock porosity (Porosity_bedrock) has dominant influence to ^{129}I annual dose throughout the 1,000,000-yr time frame. In this case, the DHLW glass degradation rate (Glass_WF_rate) shows strong influence at the earlier times while the commercial UNF degradation rate

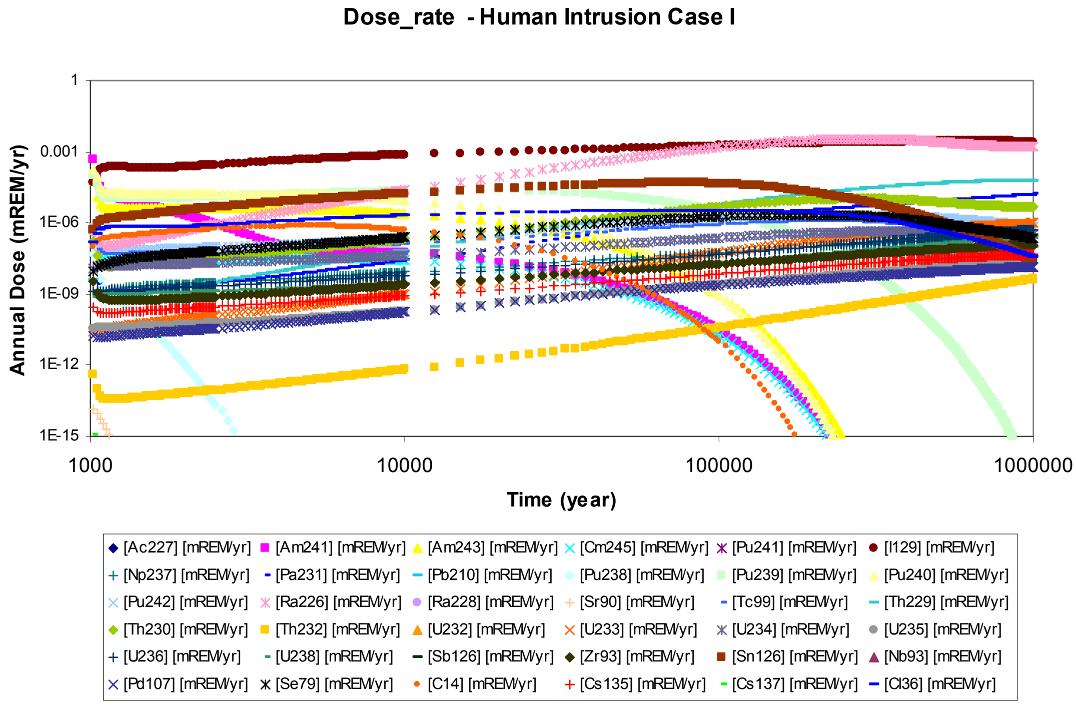


Figure 3.2-5. Disturbed Scenario: Mean Annual Dose of 100 Realizations for 36 Individual Radionuclide Species

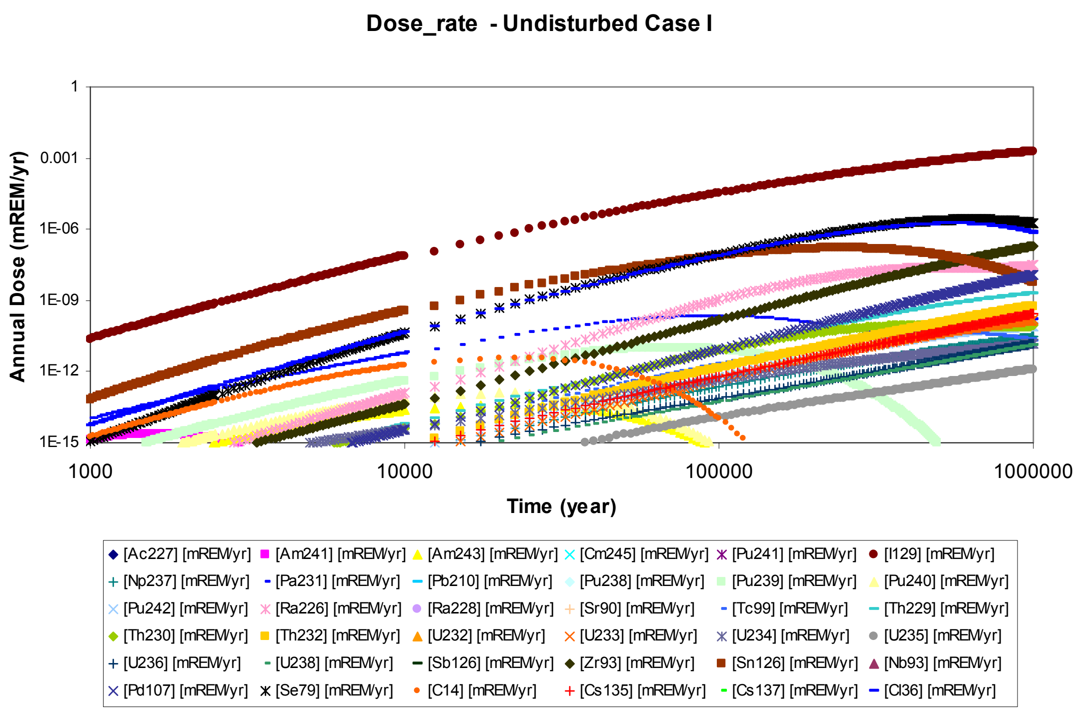
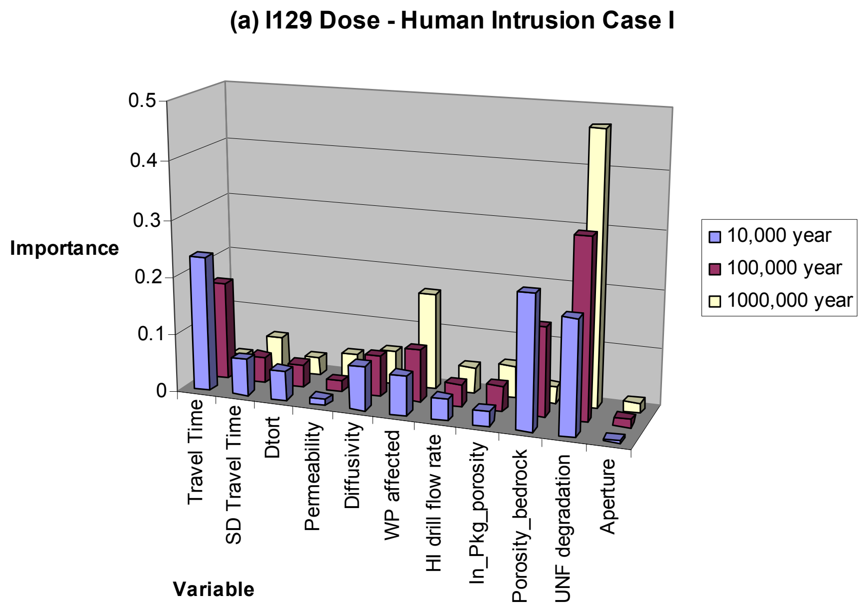
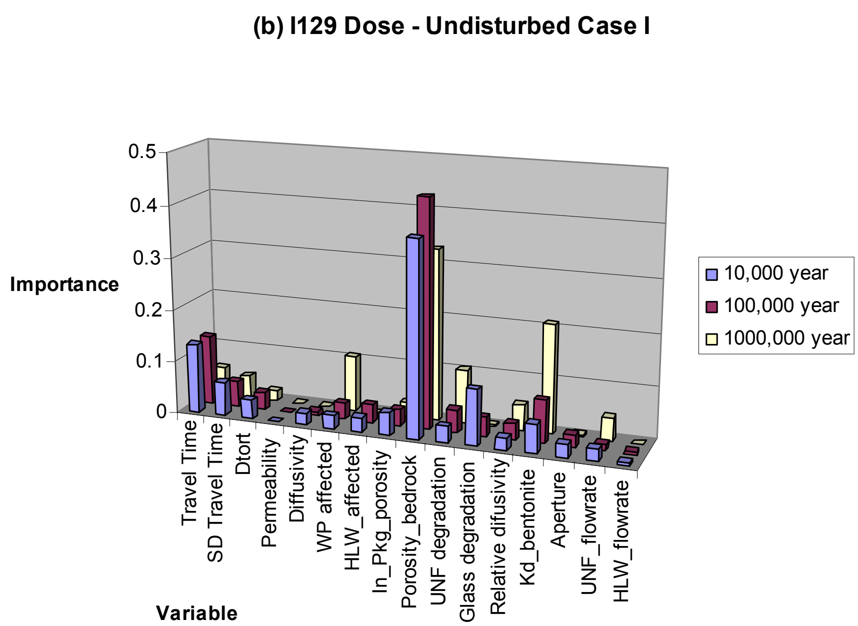


Figure 3.2-6. Undisturbed Scenario: Mean Annual Dose of 100 Realizations for 36 Individual Radionuclide Species





NOTE: Larger values for a parameter denote that the uncertainties in that parameter have a larger influence on the overall uncertainty in the ^{129}I annual dose.

Figure 3.2-7. Importance Analysis of Input Parameters with Respect to Uncertainties in the ^{129}I Annual Dose at 5-km Compliance Boundary for (a) Human Intrusion Case 1 (Commercial UNF only) and (b) Undisturbed Case 1 (Commercial UNF plus DHLW)

(UNF_WF_rate) shows strong influence toward the end of simulation. The mean travel time of water in the far field (LnorMean) has comparable influence as DHLW glass degradation rate, and its influence is also stronger at earlier times. The ^{129}I sorption coefficient for bentonite buffer (Kd_I_bentonite) shows comparable effect as the number of waste packages affected and the waste form degradation rates on the uncertainty in the annual dose, and with a relative strong influence towards the end of simulation duration.

3.2.4 Concluding Remarks

The granite GDS model and the results presented in Sections 3.2.1 through 3.2.3 are preliminary and therefore not indicative of the performance of an actual geologic disposal environment or the potential radiation exposures that could occur in that environment. Nevertheless, they can be used to identify the important processes that may affect repository performance. The intermediate applications of this model may include the following:

- Identifying which radionuclides are important to the disposal system performance;
- Determining which processes (i.e., solubility, sorption) significantly affect the disposal system performance;
- Determining how a waste form with a specific radionuclide inventory affects the disposal system performance.

Future work includes continual improvement of the existing model by incorporating more detailed physical, chemical and hydrological processes; continual improvement of the granite GDS model to enhance flexibility and integration to address technical issues with minimal changes; and performing comparative studies among the different disposal environments. These technical improvements, incorporation of increased fundamental describing the science of waste disposal in a generic granite repository, and comparative studies will occur within and using the GPAM framework, the initial version of which is described in Section 4 of this report.

3.3 Clay GDS Model

The development of the clay GDS model is discussed in the subsections of Section 3.3.

3.3.1 Introduction

The feasibility of disposing UNF and HLW in clay media has been investigated and has been shown to be promising (Hansen et al. 2010). In addition the disposal of these wastes in clay media is being investigated in Belgium, France, and Switzerland. Thus, argillaceous media is one of the environments being considered by UFD. As identified by researchers at SNL, potentially suitable formations that may exist in the United States include mudstone, clay, shale, and argillite formations (Hansen et al. 2010). These formations encompass a broad range of material properties. In this report, reference to clay media is intended to cover the full range of material properties.

Sections 3.3.1 through 3.3.5 describe the status of the development of a simulation model for evaluating the performance of generic clay media. There are multiple uses for developing this modeling capability within the UFD Campaign and the broader FCT Program:

- Inform the prioritization of R&D activities within the UFD Campaign
- Provide metric information regarding waste management that could be used by the FCT systems engineering effort in evaluating various advanced fuel cycle alternatives
- Provide metric information to the FCT System Analysis Campaign in the development of fuel cycle system analysis tools

To support these uses, the clay GDS repository performance simulation tool has been developed with the flexibility to evaluate not only different properties, but different waste streams/forms and different repository designs and engineered barrier configurations/ materials that could be used to dispose of these wastes. The capabilities of the clay GDS model are being incorporated into the GPAM (Section 4) along with the capabilities of models for the salt, granite, and deep borehole repository options. Afterwards, GPAM can be used to provide guidance on the development of strategy for long-term disposal of UNF and HLW in a clay repository.

3.3.2 Model Description

The development of a clay GDS model was initiated in FY 2009 under the FCT Separations/Waste Form Campaign (Nutt, Wang, and Lee 2009). The initial model, which focused on diffusive radionuclide transport through the far field, served as the starting point for the development of the UFD clay GDS model presented herein. Model development continued in FY 2010 under the UFD Campaign (Wang and Lee 2010), focusing on adding capabilities to model the EBS of a generic clay disposal environment. Development continued in FY 2011, resulting in the model and capabilities discussed herein. Specific enhancements included improved representation of EBS components, improved representation of the EDZ and far field, development of flexible fast pathway simulation capabilities, and additional flexibility to change parameter inputs and scenarios externally. Further development in FY 2012 and beyond will occur within the GPAM framework.

The development of the clay GDS model centered on a requirement of having the flexibility to accommodate a variety of different scenarios. These scenarios range from different material properties, different waste forms with varying radionuclide inventories, and different repository and EBS designs. As such, tool development did not begin with defining a specific scenario around which models would be developed, but rather focused on developing modeling tools that could then be used to evaluate a wide range of alternative scenarios.

The clay GDS model is envisioned primarily as a "stand-alone" tool, but includes the ability to link to external tools and ancillary calculations. The coupling of these models and their linkage to input data and the results of ancillary calculations and model output is shown in Figure 3.3-1. This report discusses the development of the clay GDS model (orange box). Other analytic tools, models, and input information are being developed within the UFD Campaign or other campaigns within the FCT Program (i.e., the Separations/Waste Form Campaign). As these tools are developed they can either be directly incorporated into future versions of the clay GDS model or can link to it, as necessary.

The objective of the clay GDS model is to integrate all of the key FEPs (Section 2 and Appendix B) for a generic clay system into an integrated framework. It is developing using the GoldSim dynamic simulation software (GoldSim Technology Group 2011), but is intended to be universally used by non-GoldSim practitioners through the use of the free GoldSim Player. All inputs are contained in an MS Excel format that is linked to the GoldSim model. This allows the user the flexibility to evaluate multiple scenarios and conduct sensitivity analyses without having to make changes to the GoldSim model itself, rather only the input needs to be changed.

The overall linkage between the clay GDS model, the input spreadsheet, and the broad FEPs categories being used by the UFD Campaign is shown in Figure 3.3-2.

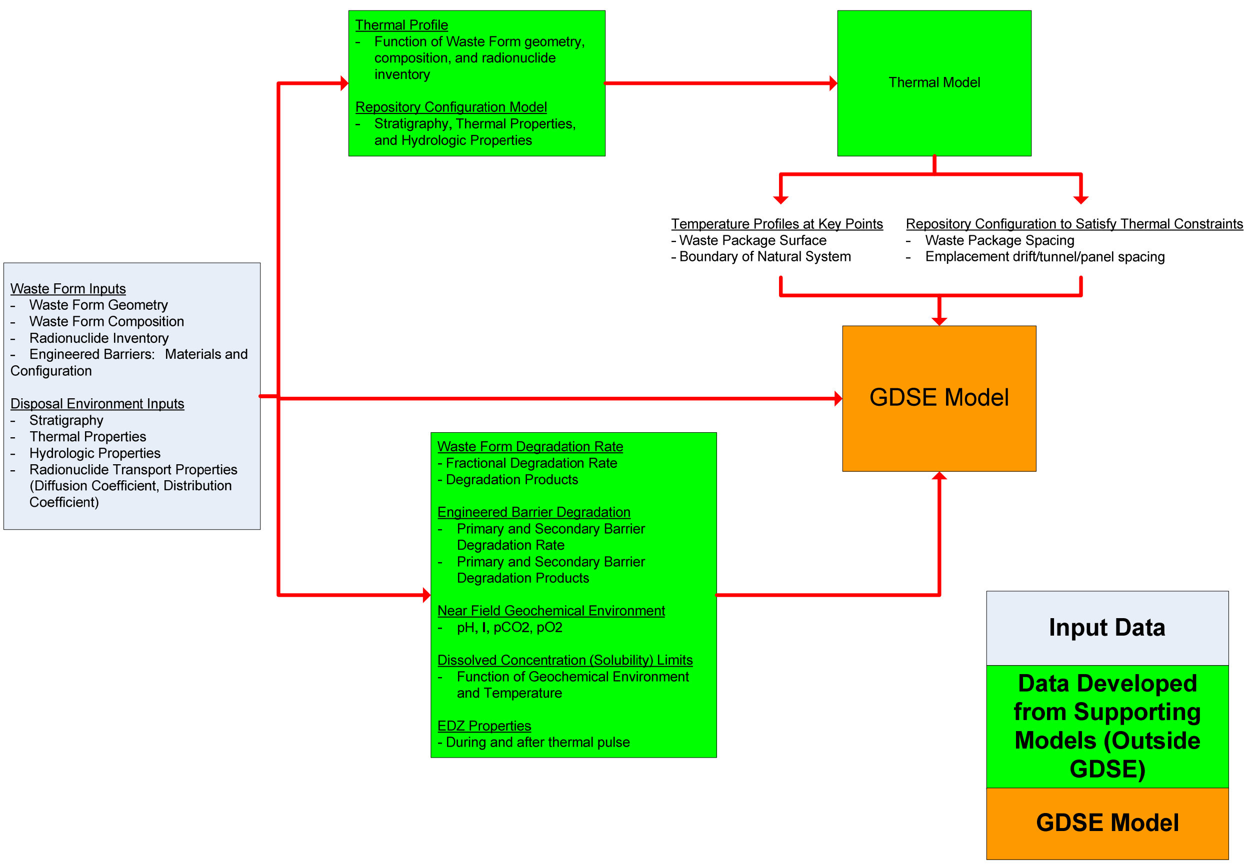
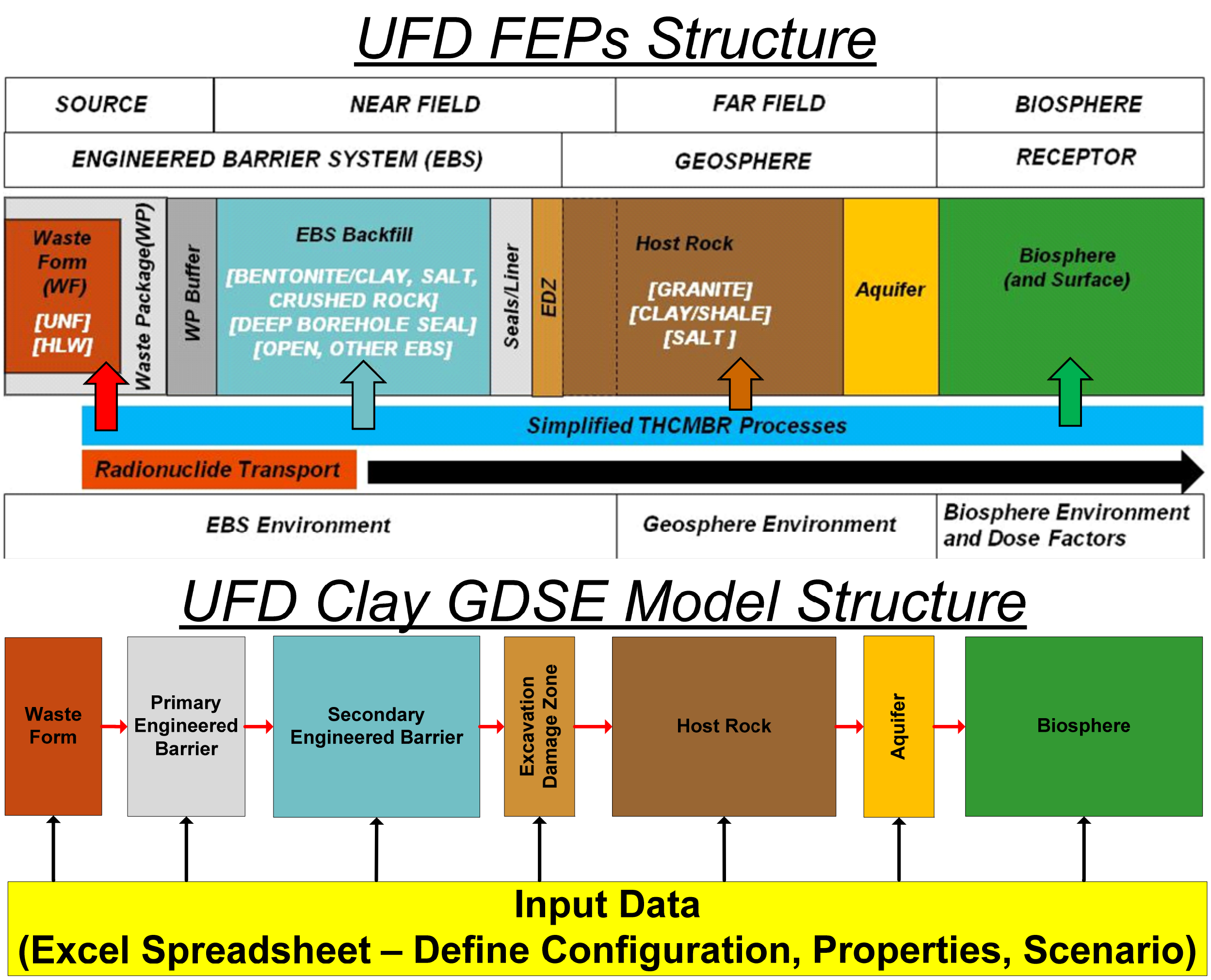


Figure 3.3-1. Clay GDS Model Structure

The general components of the clay GDS model are

- *Source Term*—Waste form and radionuclide inventory
- *Primary Engineered Barrier*—Waste package
- *Secondary Engineered Barrier*—Buffer or other material surrounding a waste package
- *EDZ*—Host rock effected by facility construction and the emplacement of waste
- *Far Field*—Host rock not affected by the emplacement of waste
- *Fast Pathways*—Generic capability to simulate the presence of fast pathways either intersecting the emplaced waste or occurring at some location within the far field (either directly intersecting the waste or the EBS, or affecting far-field transport behavior).



NOTE: For the purposes of this report, the "Excavation Damage Zone" referred to in the model structure above is considered the same as the EDZ (excavation disturbed zone).

Figure 3.3-2. Clay Long-Term Repository Performance GDS Model Linkages

3.3.2.1 Overall Model Framework

The underlying basis behind the clay GDS model is a "waste unit cell." Except near the edges, repository designs in general are repeatable configurations of emplaced waste separated by constant distances on the horizontal plane. This symmetry allows for the development of simplified 2D representations of an emplacement location and the surrounding natural media. A wide range of configurations can be modeled using the same overall modeling framework by changing input parameters. This is shown schematically in Figure 3.3-3 for different conceptualizations of waste emplacement.

The "waste unit cell" is defined by a width, height, and depth as shown in Figure 3.3-3. The clay GDS model assumes one-dimensional (1D) radionuclide transport within the EBS and 2D radionuclide transport (x – z plane in Figure 3.3-3) in the far field. The domain height (z direction in Figure 3.3-3) represents the height to an overlying conductive flow unit (an aquifer). The radionuclide concentration in the overlying aquifer is assumed to equal zero. A zero-flux boundary condition is applied at the bottom of the far-field domain, and a symmetry boundary condition (zero flux) is applied at the sides of the far-field domain.

The depth (y plane in Figure 3.3-3) represents the distance between adjacent waste emplacements and is used to determine EBS component volumes and resultant radionuclide concentrations.

In evaluating a specific site and design, more elaborate models would likely be used to evaluate 3D and asymmetric effects. However, the use of symmetrical and prescribed boundary conditions is appropriate when using simplified modeling tools to evaluate generic sites. The architecture of the GPAM, which will subsume the individual GDS models including this clay GDS model, has the flexibility to span the range of model detail from the simple to the complex.

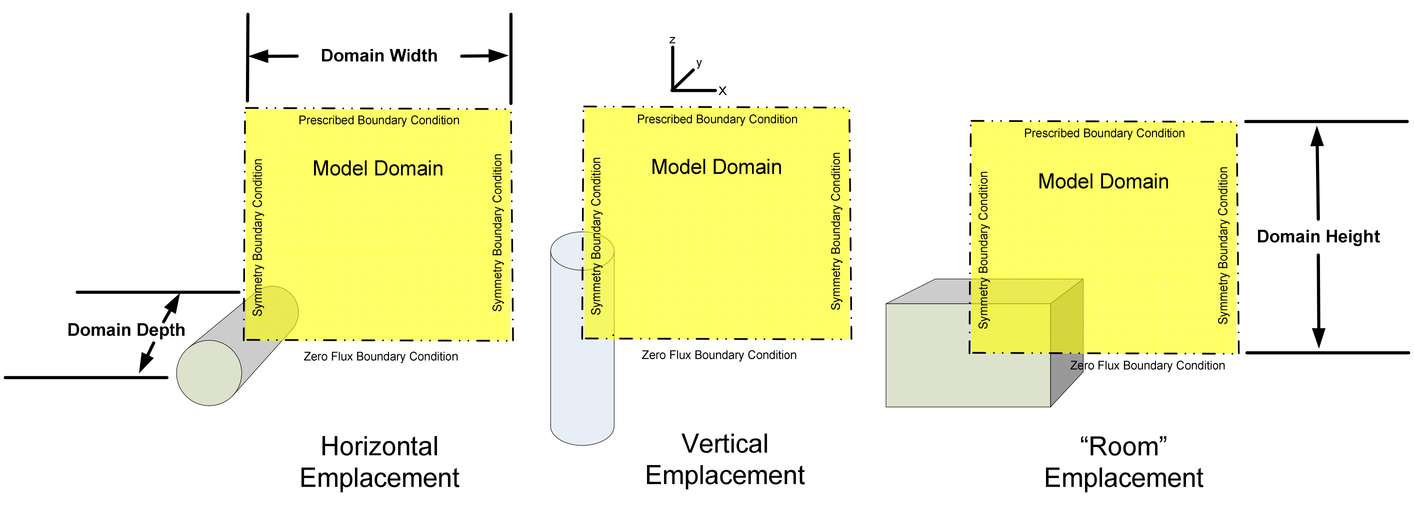


Figure 3.3-3. Conceptual Framework for Clay GDS Models

3.3.2.2 Source Term, Degraded Waste Form, Primary and Secondary Engineered Barriers

The source term, degraded waste form, and degraded primary engineered barrier components of the clay GDS model are shown schematically in Figure 3.3-4 and the secondary engineered barrier component is shown schematically in Figure 3.3-5. Also shown on these figures are the data and ancillary calculation/modeling results that serve as input to the model. As discussed previously, the user has the capability to change the input parameters through the GDS input spreadsheet and thus is able to model a wide variety of alternatives within the engineered system of a generic clay conceptual repository design.

3.3.2.2.1 Radionuclide Inventory

The source term for the clay GDS model begins with the inventory. This implementation of the model includes 36 radionuclides important to repository performance. These are input into the model from a spreadsheet as shown in Table 3.3-1 as constants that represent the inventory emplaced in a "single waste unit cell". A multiplier that can be used to conduct inventory-related sensitivity studies is also included on the input spreadsheet.

Table 3.3-1. Radionuclide Inventory

Inventory Multiplier	1.00E+00		
Isotope	**Mass (g / Waste Unit Cell)**	**Isotope**	**Mass (g / Waste Unit Cell)**
^{227}Ac	0.00E+00	^{242}Pu	1.03E+01
^{241}Am	1.81E+03	^{226}Ra	0.00E+00
^{243}Am	1.19E+03	^{228}Ra	0.00E+00
^{14}C	1.00E+00	^{126}Sb	0.00E+00
^{36}Cl	0.00E+00	^{79}Se	0.00E+00
^{245}Cm	4.21E+01	^{126}Sn	2.20E+02
^{135}Cs	3.39E+03	^{90}Sr	3.54E+03
^{137}Cs	8.19E+03	^{99}Tc	5.63E+03
^{129}I	0.00E+00	^{229}Th	2.38E-05
^{93}Nb	3.15E+03	^{230}Th	2.24E-02
^{237}Np	5.28E+03	^{232}Th	6.91E-03
^{231}Pa	0.00E+00	^{232}U	7.06E-06
^{210}Pb	0.00E+00	^{233}U	3.78E-06
^{107}Pd	0.00E+00	^{234}U	1.76E-01
^{238}Pu	1.58E+00	^{235}U	4.73E+00
^{239}Pu	2.46E+01	^{236}U	5.49E+00
^{240}Pu	6.04E+02	^{238}U	8.02E-01
^{241}Pu	3.32E+00	^{93}Zr	0.00E+00

NOTE: The inventory values shown are for example only.

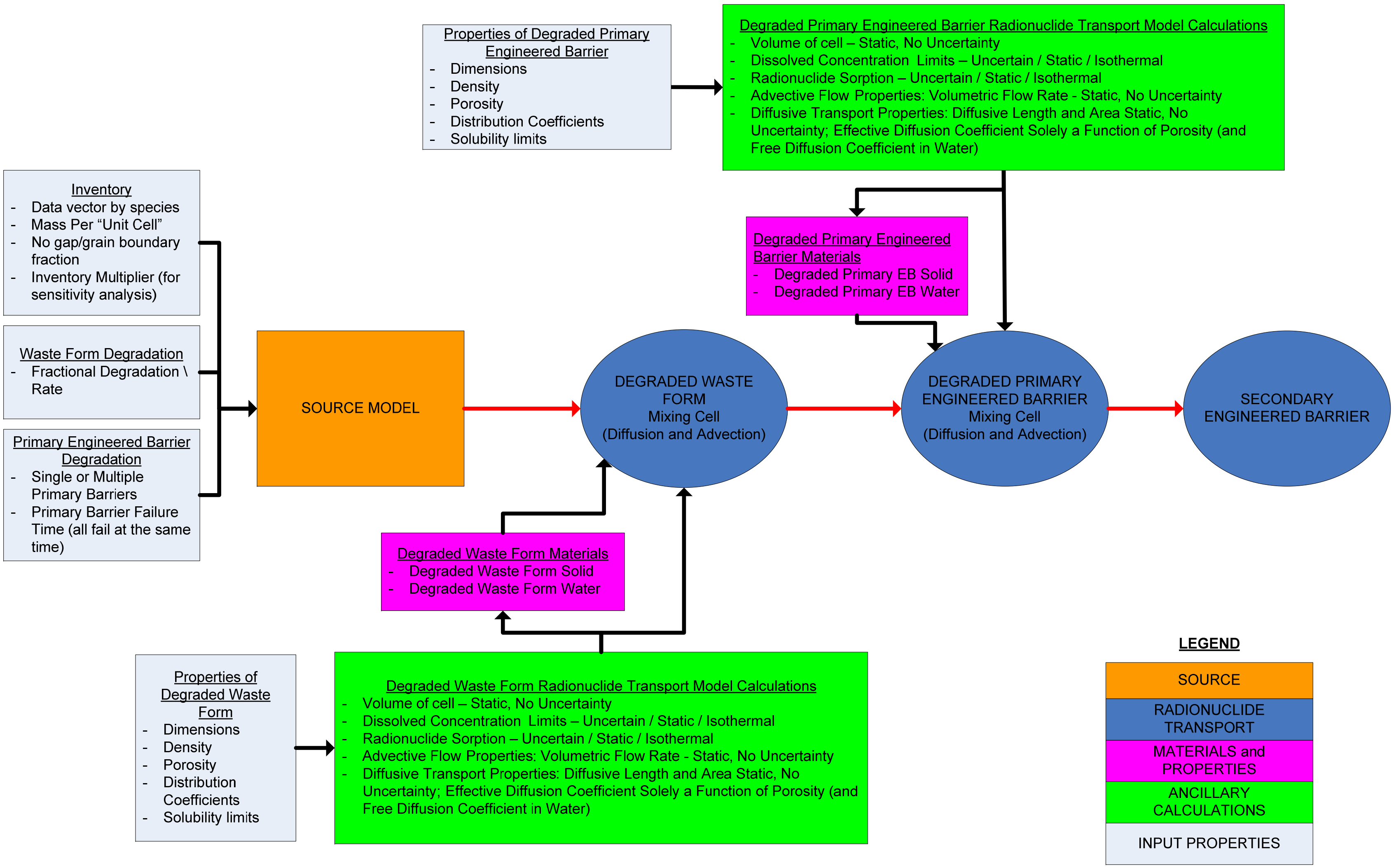


Figure 3.3-4. Schematic of Source Term, Degraded Waste Form, and Primary Engineered Barrier Representation

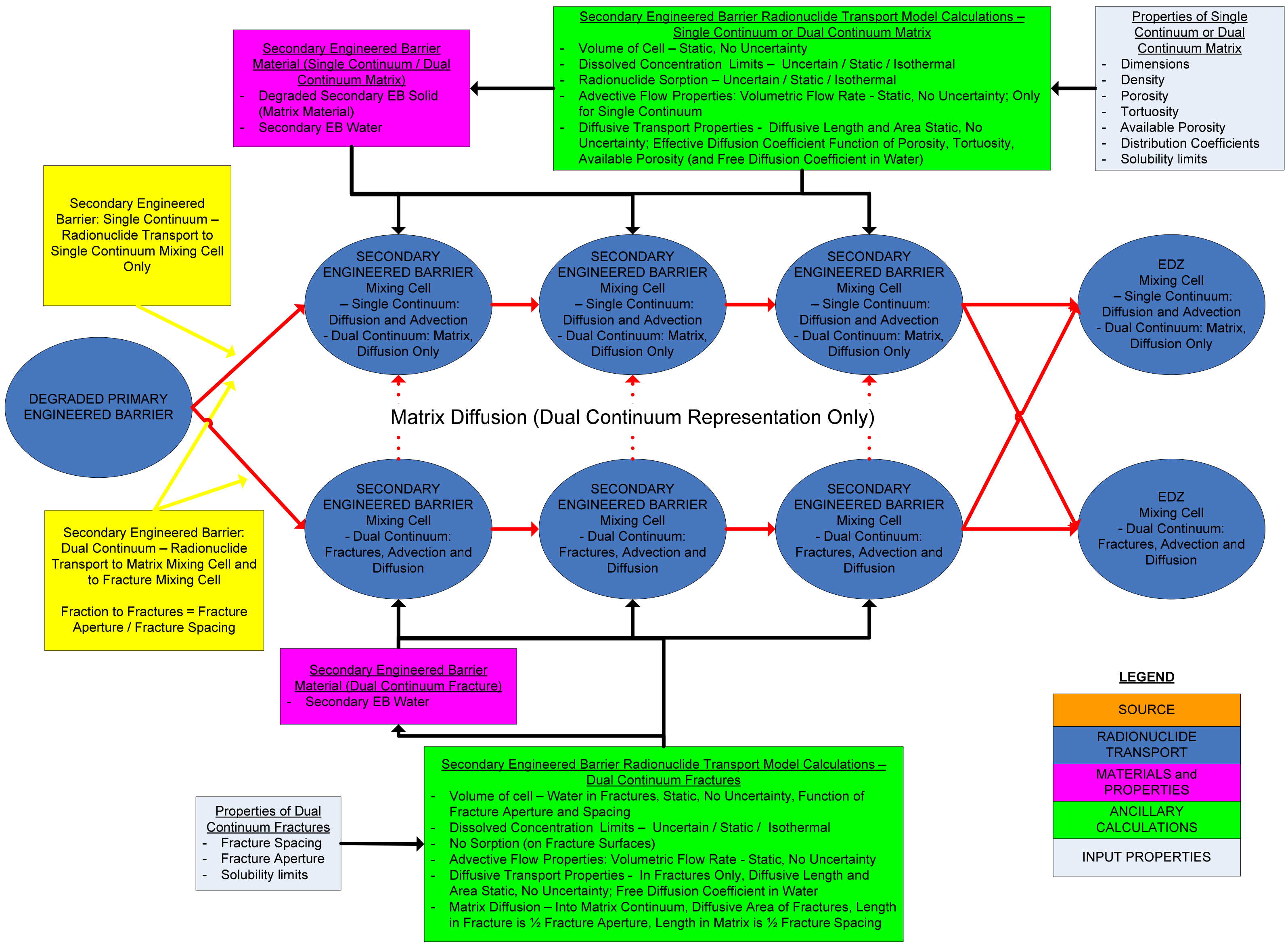


Figure 3.3-5. Schematic of Secondary Engineered Barrier Representation

3.3.2.2.2 Waste Form and Primary Engineered Barrier

The configuration of the engineered barriers is controlled from the input spreadsheet as shown in Table 3.3-2. A parameter is included to change the number of discrete units that are represented by the single "unit cell" within the clay GDS model. This allows the user to simulate the disposal of waste (with identical characteristics) at multiple identical locations within the model. The "unit cell" approach could be used to estimate the results of a full generic repository inventory through linear scaling. For example, if a scenario considers the disposal of two waste forms, two separate "unit cell" representations, one for each waste form, could be developed and executed. The resultant release and annual dose from each waste form could then be linearly scaled to the total inventory of each to provide an estimate of overall generic repository performance. It must be noted that this approach is only an approximation and does not consider any interactions between the waste packages (all assumed to behave independently).

Table 3.3-2. Waste Form and Primary Engineered Barrier Parameters

General	
Number of Discrete Units (i.e., waste packages) Represented	1
Waste Form	
Waste Form Fractional Degradation Rate (yr^{-1})	1.00E-05
Primary Engineered Barrier (i.e., Waste Package)	
Primary Engineered Barrier Present (0=no; 1=yes)	1
Waste Package Failure Time (yr)	30,000

NOTE: The values shown are for example only.

A parameter (flag) is used to define if a primary engineered barrier is included. If it is assumed that no primary barrier is present waste form degradation is assumed to immediately begin when the simulation is initiated. If a primary engineered barrier is included, its failure is represented as a single failure mode where the barrier fails completely at a defined time, exposing the waste form. If the clay GDS model is being used to represent multiple identical waste disposal locations, it is assumed that the primary engineered barrier at each of these locations fails at the same time.

The degradation of the waste form is currently represented as a single fractional degradation rate that does not vary with time. The clay GDS model assumes congruent release of all radionuclides as the waste degrades (i.e., gap/grain boundary radionuclide release from directly disposed fuel is not considered).

The clay GDS model assumes 1D radionuclide transport through the waste form and primary engineered barrier with each being modeled as single batch-reactor mixing cells. The properties of the waste form and primary engineered barrier are shown in Table 3.3-3 and are input as scalar values that do not change with time. In general, it is expected that the properties representing the fully degraded state of these barriers would be modeled; however the user can change the properties to represent different conditions.

Table 3.3-3. Waste Form and Primary Engineered Barrier Properties

Property	Waste Form	Primary Engineered Barrier
Material Density (kg/m^3)	4830	5240
Porosity	0.175	0.4
Volume (m^3)	2.6	0.400
Thickness (m)	0.40	0.03
Diffusion Area (m^2)	12.7	13.8
Advective Flow Rate (m^3/yr)	0.00E+00	0.00E+00

NOTE: The values shown are for example only.

The volume of water in each batch-reactor mixing cell is equal to the product of the volume of the cell and the porosity and the mass of solid is equal to the product of the volume of the cell and the density (assumed to be the dry density).

The batch-reactor mixing cells are both diffusively and advectively coupled. The diffusive area and length are defined by the user. The advective flow rate through the mixing cells is also defined by the user. Thus, while clay environments are expected to result primarily in diffusive transport conditions through the engineered barriers, a combination of diffusive and advective radionuclide transport can be modeled.

The diffusive area and diffusion length are input parameters as shown in Table 3.3-3. The effective diffusive coefficient is given as:

$$D_{eff,j} = D_{ref} \bullet R_{D,j} \bullet \phi \qquad \text{Eq. 3.3-1}$$

where

$D_{eff,j}$ = Effective diffusion coefficient for element j (m^2/yr)

D_{ref} = Reference diffusivity in water (m^2/yr)

$R_{D,j}$ = Relative diffusivity in water for element j

ϕ = Porosity

The reference diffusivity and the element-specific relative diffusivity in water, shown in Table 3.3-4, are user inputs (scalar values).

The ability to simulate dissolution/precipitation and reversible sorption is included in each batch-reactor mixing cell. It is assumed that the dissolved concentration limits and distribution coefficients are

Table 3.3-4. Reference and Relative Diffusivity

Radioelement	Relative Diffusivity	Radioelement	Relative Diffusivity
Ac	1.000	Pd	1.000
Am	0.413	Pu	0.565
C	0.513	Ra	0.387
Cl	0.883	Sb	1.000
Cm	1.000	Se	0.452
Cs	0.896	Sn	0.674
I	0.892	Sr	0.344
Nb	1.000	Tc	0.848
Np	0.269	Th	0.260
Pa	0.263	U	0.289
Pb	1.000	Zr	1.000
Reference Diffusivity ($m^2 s^{-1}$)		2.30E-09	

NOTE: The values shown are for example only.

represented in the clay GDS model as log-triangular, as shown in Table 3.3-5, with the user having the ability to define the minimum, best estimate, and maximum values of the distribution from the input spreadsheet for the waste form and primary engineered barrier (separate input tables for each barrier).

For scenarios where the degraded waste form, the degraded primary engineered barrier, are not part of the specific option being simulated, these barriers can be by-passed by an appropriate choice of parameter values can be defined to force immediate transport through the mixing cells by:

- Setting the cell volumes to a very small number (i.e. 10^{-5} m^3);
- Setting the advective flow rate out of the mixing cell to a very large number (i.e. 10^{10} m^3/yr)
- Setting the dissolved concentration limit to a very large number (i.e. 10^{50} mol/L)
- Setting the distribution coefficients for each element to a very small number (i.e. 10^{-50} m^3/kg)

3.3.2.2.3 Secondary Engineered Barrier

The clay GDS model currently assumes 1D radionuclide transport through the secondary engineered barrier using the linked batch-reactor mixing cell structure shown in Figure 3.3-5. This structure allows the user to select either a single- or a dual-continuum representation of radionuclide transport. This allows for the representation of a variety of secondary engineered barrier materials (i.e., bentonite or cementitious) with different radionuclide transport properties.

If a single-continuum representation is chosen, radionuclide transport through the secondary engineered barrier is represented by three linked batch-reactor mixing cells (top cell network shown in Figure 3.3-5) that span the thickness of the barrier. It is assumed that diffusion is the primary radionuclide transport mechanism in a clay disposal environment, so the batch-reactor mixing cells are diffusively coupled. However, to investigate the effects of advective transport through the engineered barriers, the mixing cells are also advectively linked with the model user able to input an advective flow rate.

Table 3.3-5. Dissolved Concentration Limit and Distribution Coefficient Parameters (Log-triangular Distribution)

Element	Dissolved Concentration Limit (Mol/L)			Distribution Coefficient (m^3/Kg)		
	Minimum	Most Likely	Maximum	Minimum	Most Likely	Maximum
Actinium	4.00E-09	2.00E-06	2.00E-05	1.00E+00	5.00E+00	5.00E+00
Americium	3.00E-10	2.00E-09	1.00E-08	1.00E+00	5.00E+00	5.00E+00
Antimony	1.00E+50	1.00E+50	1.00E+50	1.00E-51	1.00E-50	1.00E-49
Carbon	9.70E-06	2.00E-04	2.00E-04	1.00E-02	1.00E-01	1.00E-01
Cesium	1.00E+50	1.00E+50	1.00E+50	1.00E-51	3.00E-01	3.00E-01
Chlorine	1.00E+50	1.00E+50	1.00E+50	1.00E-51	1.00E-50	1.00E-49
Curium	3.00E-10	2.00E-09	1.00E-08	1.00E-51	1.00E-50	1.00E-49
Iodine	1.00E+50	1.00E+50	1.00E+50	1.00E-51	1.00E-50	1.00E-49
Lead	3.00E-03	2.00E-02	2.00E-02	1.00E-51	1.00E-50	1.00E-49
Neptunium	3.00E-09	5.00E-09	1.00E-08	5.00E-01	1.00E+00	1.00E+00
Niobium	1.00E+50	1.00E+50	1.00E+50	1.00E-51	1.00E-50	1.00E-49
Paladium	8.00E-08	8.00E-07	8.00E-06	1.00E-51	1.00E-50	1.00E-49
Protactinium	1.00E-09	1.00E-08	1.00E-07	5.00E-01	1.00E+00	1.00E+00
Plutonium	1.00E-11	4.00E-11	2.00E-10	1.00E+00	5.00E+00	5.00E+00
Radium	1.00E-06	2.00E-02	2.00E-01	1.00E-51	5.00E-01	5.00E-01
Selenium	7.00E-06	1.00E-05	2.00E-05	1.00E-51	1.00E-50	1.00E-49
Strontium	1.00E-03	6.00E-03	6.01E-03	1.00E-51	2.00E-02	2.00E-02
Technetium	3.20E-07	1.00E-04	1.00E-04	1.00E-51	1.00E-50	1.00E-49
Thorium	8.00E-10	3.00E-09	1.00E-08	1.00E+00	5.00E+00	5.00E+00
Tin	1.00E-07	2.00E-07	2.00E-07	1.00E-51	1.00E-50	1.00E-49
Uranium	1.00E-08	5.00E-07	5.01E-07	1.00E-01	1.00E+00	1.00E+00
Zirconium	6.00E-07	6.00E-05	6.01E-05	1.00E-51	1.00E-50	1.00E-49

NOTE: The values shown are for example only.

If a dual-continuum representation is chosen, radionuclide transport through the secondary engineered barrier is represented by six linked batch-reactor mixing cells (shown in Figure 3.3-5). Three of the linked batch-reactor mixing cells (top cell network shown in Figure 3.3-5), that span the thickness of the barrier, represent the matrix continuum and three of the batch-reactor mixing cells (bottom cell network shown in Figure 3.3-5) represent the fracture continuum. The batch-reactor mixing cells are both diffusively and advectively coupled. The diffusive area and length are defined by the user. The advective flow rate through the mixing cells is also defined by the user. Thus, while clay environments are expected to result primarily in diffusive transport conditions through the engineered barriers, a combination of diffusive and advective radionuclide transport can be modeled.

The diffusion of radionuclides between the matrix and fracture continua is also included in the dual-continuum representation. To investigate the effects of advective transport through the engineered barriers, the dual-continuum representation advectively links the fracture cell network with the user able to input an advective flow rate. No advective flow through the matrix continua occurs in the dual-continuum representation.

The properties of the secondary engineered barrier are shown in Table 3.3-6. The volume, thickness, and perimeter of the secondary engineered barrier are input as scalar values and the porosity, density, tortuosity, fracture spacing, and fracture aperture are represented by log-triangular probability distributions. The properties also do not change with time. In general, it is expected that properties associated with the fully degraded state of the secondary engineered barrier would be modeled; however the user can change the properties to represent different conditions.

The ability to simulate dissolution/precipitation and reversible sorption is included in each secondary engineered barrier batch-reactor mixing cell. It is assumed that the dissolved concentration limits and distribution coefficients are represented in the clay GDS model as log-triangular, as shown in Table 3.3-5, with the user having the ability to define the minimum, best estimate, and maximum values of the distribution from the input spreadsheet for the secondary engineered barrier.

Single-Continuum Representation

In this model version, the single-continuum representation of the volume of water in each batch-reactor mixing cell is equal to the product of the 1/3rd the volume of the secondary engineered barrier and the porosity (3 mixing cells). The mass of solid material in the mixing cell is equal to the product of 1/3rd the volume of the secondary engineered barrier and the density (assumed to be the dry density).

For the single-continuum representation, 1D diffusive radionuclide transport is modeled assuming the diffusive area is equal to the product of the outer perimeter of the secondary engineered barrier and the model domain depth (Figure 3.3-3). This diffusive area is applied to all three batch reactor mixing cells, resulting in a larger diffusive area than would result from a more explicit representation of the geometry. However, this approach will result in larger diffusive fluxes and is a conservative approximation. The diffusive length in each batch-reactor mixing cell is equal to 1/3rd the thickness of the secondary engineered barrier.

The effective diffusion coefficient is given as:

$$D_{eff,j} = D_{ref} \bullet R_{D,j} \bullet \phi \bullet \tau \bullet \phi_{A,j} \qquad \text{Eq. 3.3-2}$$

where

$D_{eff,j}$	=	Effective diffusion coefficient for element j (m^2/yr)
D_{ref}	=	Reference diffusivity in water (m^2/yr); Table 3.3-4
$R_{D,j}$	=	Relative diffusivity in water for element j; Table 3.3-4
ϕ	=	Porosity
τ	=	Tortuosity
$\phi_{A,j}$	=	Available porosity for element j (0-1); Table 3.3-7

This approach for determining the effective diffusion coefficient provides flexibility to the user in representing diffusive radionuclide transport in the single-continuum representation of the secondary engineered barrier. As discussed above, both the reference diffusivity and the element-specific relative diffusivities in water are user inputs (Table 3.3-4). The element-specific available porosities are represented as triangular distributions with the minimum, most likely, and maximum values being user inputs, as shown in Table 3.3-7.

Table 3.3-6. Secondary Engineered Barrier Properties

(a) Scalar Parameters

Property	Secondary Engineered Barrier
Volume (m^3)	18.0
Thickness (m)	0.6
Perimeter (m)	40
Advective Flow Rate (m^3/yr)	0.00E+00

(b) Stochastic Parameters

Property	Minimum	Most Likely	Maximum
Porosity	0.05	0.1	0.15
Density (kg/m^3)	1971	2190	2409
Tortuosity	0.75	0.9	1
Fracture Spacing (m)	0.225	2.50E-01	0.275
Fracture Aperture (m)	0.004	0.005	0.006

NOTE: The values shown are for example only. Fracture Spacing and Fracture Aperture are required only for a dual-continuum representation.

Table 3.3-7. Available Porosity

Element	Minimum	Most Likely	Maximum	Element	Minimum	Most Likely	Maximum
Ac	0.998	0.999	1	Pd	0.998	0.999	1
Am	0.998	0.999	1	Pu	0.998	0.999	1
C	0.998	0.999	1	Ra	0.998	0.999	1
Cl	0.998	0.999	1	Sb	0.998	0.999	1
Cm	0.998	0.999	1	Se	0.998	0.999	1
Cs	0.998	0.999	1	Sn	0.998	0.999	1
I	0.998	0.999	1	Sr	0.998	0.999	1
Nb	0.998	0.999	1	Tc	0.998	0.999	1
Np	0.998	0.999	1	Th	0.998	0.999	1
Pa	0.998	0.999	1	U	0.998	0.999	1
Pb	0.998	0.999	1	Zr	0.998	0.999	1

NOTE: The values shown are for example only.

Dual-Continuum Representation

In this model version, the volume of water in the batch-reactor mixing cells that represent the matrix continuum, the mass of solid material in the mixing cell, the diffusive area, the diffusive length, and the effective diffusion coefficient are determined identical to the single-continuum representation discussed immediately above.

The conceptual representation of the fracture-continuum assumes equally spaced, through-going, parallel fractures along the outer perimeter of the secondary engineered barrier, as shown schematically in Figure 3.3-6.

The volume of water in the batch-reactor mixing cells that represent the fracture continuum is determined as:

$$V_W = \frac{P_{SEC\,EB}}{F_s} \bullet F_A \bullet \frac{T_{SEC\,EB}}{3} \bullet D_{domain} \qquad \text{Eq. 3.3-3}$$

where

V_W	=	Volume of water in a fracture continuum batch-reactor mixing cell (m^3)
$P_{SEC\,EB}$	=	Outer perimeter of the secondary engineered barrier (m)
$T_{SEC\,EB}$	=	Thickness of the secondary engineered barrier (m); factor of three applied since there are three batch-reactor mixing cells spanning the thickness
F_S	=	Fracture spacing along the outer perimeter of the secondary engineered barrier (m)
F_A	=	Fracture aperture (m)
D_{Domain}	=	Model domain depth (m); Figure 3.3-3

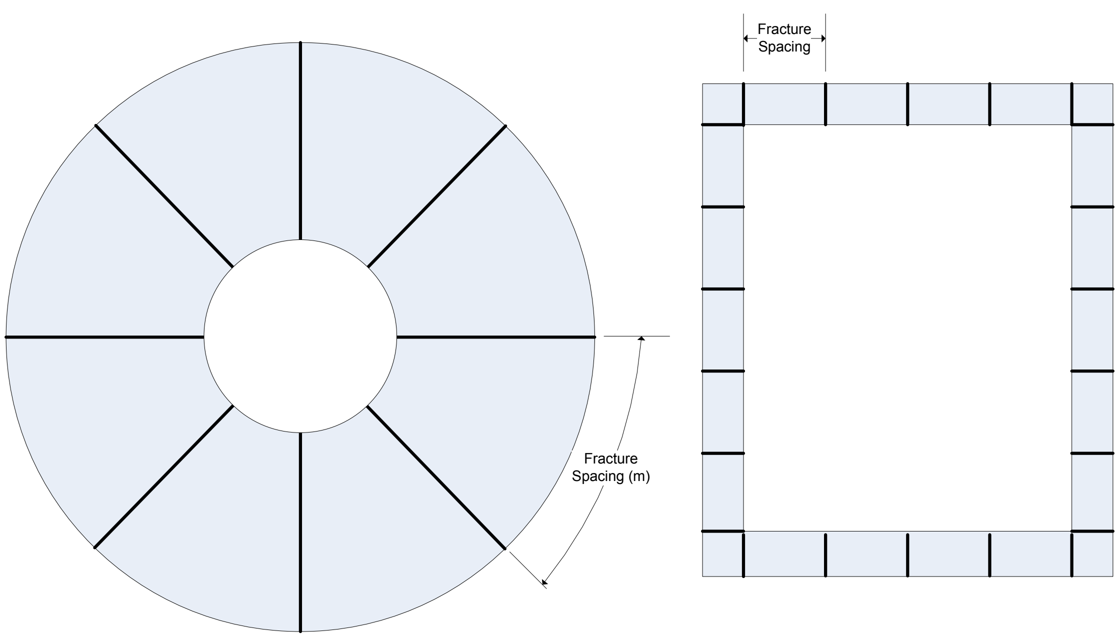


Figure 3.3-6. Schematic of Fracture Network Representation in the Secondary Engineered Barrier

The diffusive length within each fracture-continua cell is equal to 1/3rd the thickness of the secondary engineered barrier and the diffusive area is determined as:

$$D_{A-F} = \frac{P_{SEC\,EB}}{F_s} \bullet F_A \bullet D_{domain} \qquad \text{Eq. 3.3-4}$$

where

$D_{A\text{-}F}$	=	Diffusive area in a fracture continuum batch-reactor mixing cell (m^2)
$P_{SEC\,EB}$	=	Outer perimeter of the secondary engineered barrier (m)
F_S	=	Fracture spacing along the outer perimeter of the secondary engineered barrier (m)
F_A	=	Fracture aperture (m)
D_{Domain}	=	Model domain depth (m); Figure 3.3-3

The diffusive area between the fracture and matrix continuums (matrix diffusion) is determined as:

$$D_{A-M} = \frac{P_{SEC\,EB}}{F_s} \bullet 2 \bullet \frac{T_{SEC\,EB}}{3} \bullet D_{domain} \qquad \text{Eq. 3.3-5}$$

where

$D_{A\text{-}M}$	=	Diffusive area for matrix diffusion between the fracture and matrix continuum batch-reactor mixing cells (m^2)
$P_{SEC\,EB}$	=	Outer perimeter of the secondary engineered barrier (m)
$T_{SEC\,EB}$	=	Thickness of the secondary engineered barrier (m); factor of three applied since there are three batch-reactor mixing cells spanning the thickness, 2 surfaces for each fracture
F_S	=	Fracture spacing along the outer perimeter of the secondary engineered barrier (m)
D_{Domain}	=	Model domain depth (m); Figure 3.3-3

The diffusive length in the fracture continua batch-reactor mixing cell is assumed to be zero meters. The diffusive length in the matrix continua batch-reactor mixing cell is assumed to equal half the fracture spacing.

The effective diffusive coefficient in the water with the fracture continua batch-reactor mixing cells is given as:

$$D_{eff,j} = D_{ref} \bullet R_{D,j} \qquad \text{Eq. 3.3-6}$$

where

$D_{eff,j}$	=	Effective diffusion coefficient for element j (m^2/yr)
D_{ref}	=	Reference diffusivity in water (m^2/yr); Table 3.3-4
$R_{D,j}$	=	Relative diffusivity in water for element j; Table 3.3-4

For scenarios where the secondary engineered barrier is not considered, parameters in the input spreadsheet can be defined to force immediate transport through the mixing cells by:

- Selecting single-continuum for representing radionuclide transport
- Setting the cell volumes to a very small number (i.e. 10^{-5} m^3);
- Setting the advective flow rate out of the mixing cell to a very large number (i.e. 10^{10} m^3/yr)
- Setting the dissolved concentration limit to a very large number (i.e. 10^{50} mol/L)
- Setting the distribution coefficients for each element to a very small number (i.e. 10^{-50} m^3/kg)

3.3.2.3 Near Field / EDZ

The current near-field/EDZ component of the clay GDS model is shown schematically in Figure 3.3-7. Also shown are the data and ancillary calculation/modeling results that serve as input to the model. As discussed previously, the user has the capability to change the input parameters through the GDS input spreadsheet and thus is able to model a wide variety of near-field/EDZ conditions within generic clay media.

The current clay GDS model assumes 1D radionuclide transport through the secondary engineered barrier using the linked batch-reactor mixing cell structure shown in Figure 3.3-7. This structure allows the user to select either a single- or a dual-continuum representation of radionuclide transport. This allows for the representation of a variety of EDZ conditions with different radionuclide transport properties.

If a single-continuum representation is chosen, radionuclide transport through the EDZ is represented by three linked batch-reactor mixing cells (top cell network shown in Figure 3.3-7) that span the EDZ thickness. Diffusion is the primary radionuclide transport mechanism in a clay disposal environment, so the batch-reactor mixing cells are diffusively coupled. However, to investigate the effects of advective transport through the engineered barriers, the mixing cells are also advectively linked with the model user able to input an advective flow rate.

If a dual-continuum representation is chosen, radionuclide transport through the EDZ is represented by six linked batch-reactor mixing cells (shown in Figure 3.3-7). Three of the linked batch-reactor mixing cells (top cell network shown in Figure 3.3-7), that span the thickness of the EDZ, represent the matrix continuum and three of the batch-reactor mixing cells (bottom cell network shown in Figure 3.3-7) represent the fracture continuum. Again, diffusion is the primary radionuclide transport mechanism in a clay disposal environment, so the batch-reactor mixing cells representing the fracture continuum are diffusively coupled. The diffusion of radionuclides between the matrix and fracture continua is also included in the dual-continuum representation. To investigate the effects of advective transport through the engineered barriers, the dual-continuum representation advectively links the fracture cell network with the user able to input an advective flow rate. No advective flow through the matrix continua occurs in the dual-continuum representation.

The properties of the secondary engineered barrier are shown in Table 3.3-8. The volume, thickness, and perimeter of the EDZ are input as scalar values and the porosity, density, tortuosity, fracture spacing, and fracture aperture are represented by log-triangular probability distributions. The properties also do not change with time. In general, it is expected that the fully degraded state of the EDZ would be modeled; however the user can change the properties to represent different conditions.

The ability to simulate dissolution/precipitation and reversible sorption is included in each EDZ barrier batch-reactor mixing cell of the current model version. It is assumed that the dissolved concentration limits and distribution coefficients are represented in the current clay GDS model as log-triangular, as shown in Table 3.3-4, with the user having the ability to define the minimum, best estimate, and maximum values of the distribution from the input spreadsheet for the secondary engineered barrier.

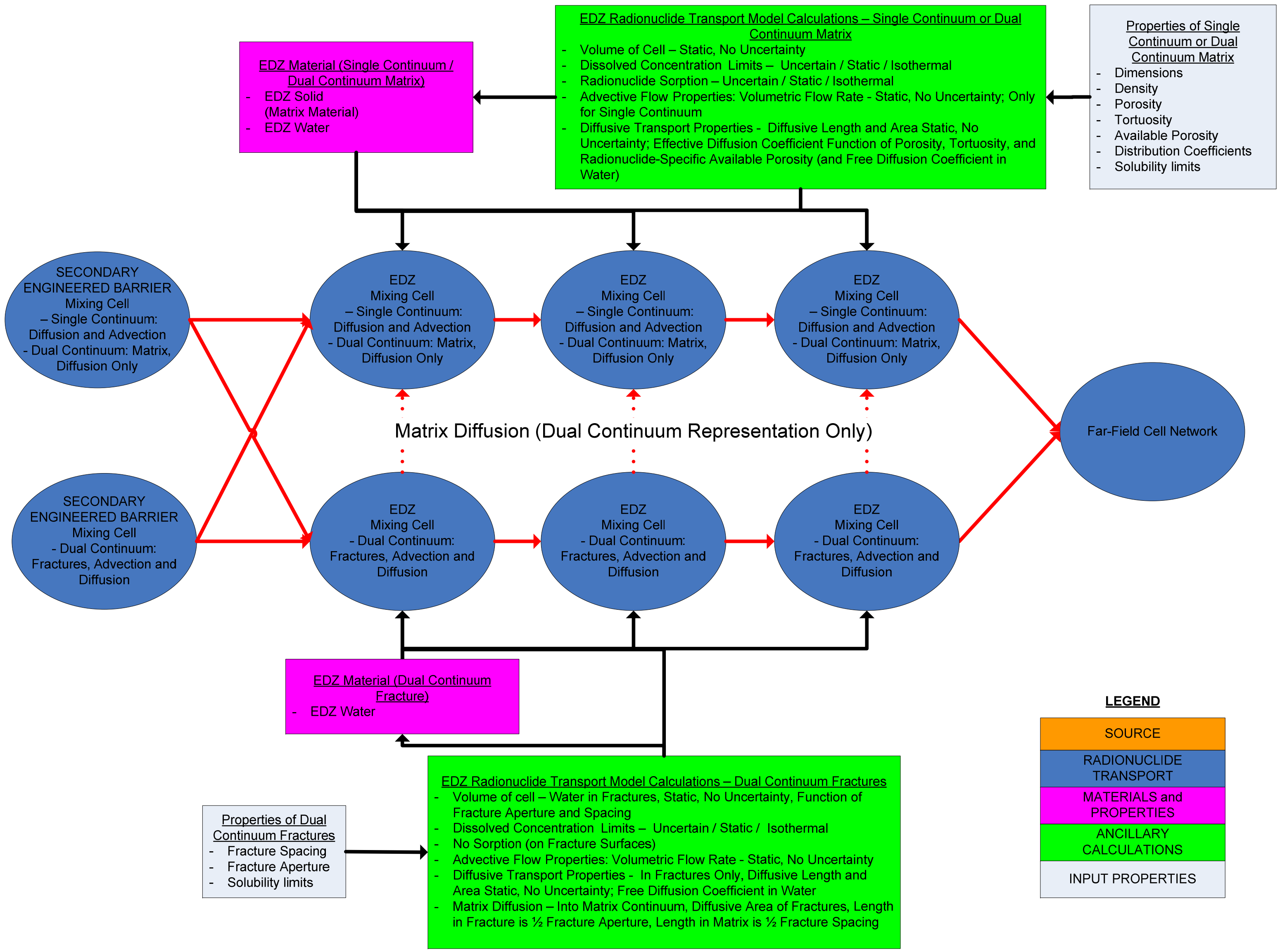


Figure 3.3-7. Schematic of Near-Field/EDZ Representation

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Table 3.3-8. EDZ Properties

(a) Scalar Parameters

Property	EDZ
Volume (m^3)	270
Thickness (m)	1.15
Perimeter (m)	6.9
Advective Flow Rate (m^3/yr)	2.8E-06

(b) Stochastic Parameters

Property	Minimum	Most Likely	Maximum
Porosity	0.15	0.18	0.20
Density(kg/m^3)	2000	2250	2500
Tortuosity	0.5	0.75	1.0
Fracture Spacing (m)	0.25	0.5	1
Fracture Aperture (m)	0.0005	0.001	0.005

NOTE: The values shown are for example only. Fracture Spacing and Fracture Aperture are required only for a dual-continuum representation.

3.3.2.3.1 Single-Continuum Representation

In the current model version, the single-continuum representation of the volume of water in each batch-reactor mixing cell is equal to the product of the 1/3rd the volume of the EDZ and the porosity (3 mixing cells). The mass of solid material in the mixing cell is equal to the product of 1/3rd the volume of the EDZ and the density (assumed to be the dry density).

For the single-continuum representation, 1D diffusive radionuclide transport is modeled assuming the diffusive area is equal to the product of the outer perimeter of the EDZ and the model domain depth (Figure 3.3-3). This diffusive area is applied to all three batch reactor mixing cells, resulting in a larger diffusive area than would result from a more explicit representation of the geometry. However, this approach will result in larger diffusive fluxes and is a conservative approximation. The diffusive length in each batch-reactor mixing cell is equal to 1/3rd the thickness of the EDZ.

The effective diffusion coefficient is given as:

$$D_{eff,j} = D_{ref} \bullet R_{D,j} \bullet \phi \bullet \tau \bullet \phi_{A,j} \qquad \text{Eq. 3.3-7}$$

where

$D_{eff,j}$	=	Effective diffusion coefficient for element j (m^2/yr)
D_{ref}	=	Reference diffusivity in water (m^2/yr); Table 3.3-4
$R_{D,j}$	=	Relative diffusivity in water for element j; Table 3.3-4
ϕ	=	Porosity
τ	=	Tortuosity
$\phi_{A,j}$	=	Available porosity for element j (0 – 1); Table 3.3-7

This approach for determining the effective diffusion coefficient provides flexibility to the user in representing diffusive radionuclide transport in the single-continuum representation of the EDZ. As discussed above, both the reference diffusivity and the element-specific relative diffusivities are user inputs. The element-specific available porosities are represented as triangular distributions with the minimum, most likely, and maximum values being user inputs, as shown in Table 3.3-7 (identical input table for the EDZ).

3.3.2.3.2 Dual-Continuum Representation

The volume of water in the batch-reactor mixing cells that represent the matrix continuum, the mass of solid material in the mixing cell, the diffusive area, the diffusive length, and the effective diffusion coefficient are determined identical to the single-continuum representation discussed immediately above.

The conceptual representation of the fracture-continuum assumes equally spaced, through-going, parallel fractures along the outer perimeter of the EDZ, as shown schematically in Figure 3.3-6.

The volume of water in the batch-reactor mixing cells that represent the fracture continuum is determined as:

$$V_W = \frac{P_{EDZ}}{F_s} \bullet F_A \bullet \frac{T_{EDZ}}{3} \bullet D_{domain} \qquad \text{Eq. 3.3-8}$$

where

V_W	=	Volume of water in a fracture continuum batch-reactor mixing cell (m^3)
P_{EDZ}	=	Outer perimeter of the EDZ (m)
T_{EDZ}	=	Thickness of the EDZ (m); factor of three applied since there are three batch-reactor mixing cells spanning the thickness
F_S	=	Fracture spacing along the outer perimeter of the EDZ (m)
F_A	=	Fracture aperture (m)
D_{Domain}	=	Model domain depth (m); Figure 3.3-3

The diffusive length within each fracture-continua cell across the thickness of the EDZ is equal to $1/3^{rd}$ the thickness. The diffusive area perpendicular to the fracture network is determined as:

$$D_{A-F} = \frac{P_{EDZ}}{F_s} \bullet F_A \bullet D_{domain} \qquad \text{Eq. 3.3-9}$$

where

D_{A-F}	=	Diffusive area in a fracture continuum batch-reactor mixing cell (m^2)
P_{EDZ}	=	Outer perimeter of the secondary engineered barrier (m)
F_S	=	Fracture spacing along the outer perimeter of the secondary engineered barrier (m)
F_A	=	Fracture aperture (m)
D_{Domain}	=	Model domain depth (m); Figure 3.3-3

The representation of matrix diffusion between the fracture and matrix continuums (matrix diffusion) determines the diffusive area as:

$$D_{A-M} = \frac{P_{EDZ}}{F_s} \bullet 2 \bullet \frac{T_{EDZ}}{3} \bullet D_{domain} \qquad \text{Eq. 3.3-10}$$

where

$D_{A\text{-}M}$	=	Diffusive area for matrix diffusion between the fracture and matrix continuum batch-reactor mixing cells (m^2)
P_{EDZ}	=	Outer perimeter of the secondary engineered barrier (m)
T_{EDZ}	=	Thickness of the secondary engineered barrier (m); factor of three applied since there are three batch-reactor mixing cells spanning the thickness, 2 surfaces for each fracture
F_S	=	Fracture spacing along the outer perimeter of the secondary engineered barrier (m)
D_{Domain}	=	Model domain depth (m); Figure 3.3-3

The matrix representation also assumes that the diffusive length in the fracture continua batch-reactor mixing cell is zero meters and the diffusive length in the matrix continua batch-reactor mixing cell is equal to half the fracture spacing.

The effective diffusive coefficient in the water with the fracture continua batch-reactor mixing cells is given as:

$$D_{eff,j} = D_{ref} \bullet R_{D,j} \qquad \text{Eq. 3.3-11}$$

where

$D_{eff,j}$	=	Effective diffusion coefficient for element j (m^2/yr)
D_{ref}	=	Reference diffusivity in water (m^2/yr); Table 3.3-4
$R_{D,j}$	=	Relative diffusivity in water for element j; Table 3.3-4

This effective diffusion coefficient is used to both represent 1D diffusion along the fracture network and matrix diffusion with the water-containing fracture, perpendicular to the fracture network. The effective diffusion coefficient for representing matrix diffusion perpendicular to the fracture network within the matrix continuum is determined identical to the single-continuum representation discussed immediately above.

For scenarios where the EDZ is not considered, parameters in the input spreadsheet can be defined to force immediate transport through the mixing cells by:

- Selecting single-continuum for representing radionuclide transport
- Setting the cell volumes to a very small number (i.e. 10^{-5} m^3);
- Setting the advective flow rate out of the mixing cell to a very large number (i.e. 10^{10} m^3/yr)
- Setting the dissolved concentration limit to a very large number (i.e. 10^{50} mol/L)
- Setting the distribution coefficients for each element to a very small number (i.e. 10^{-50} m^3/kg)

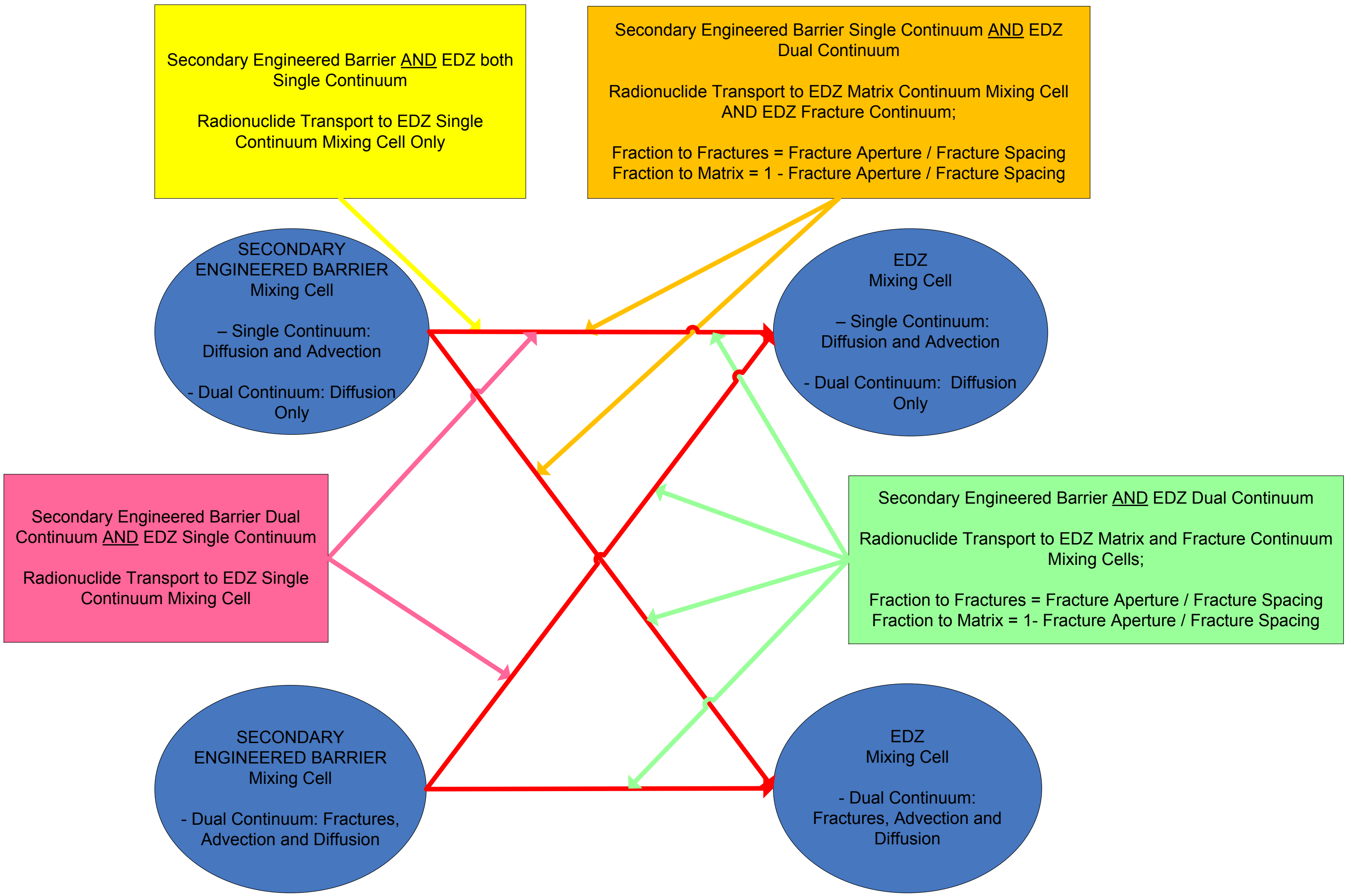


Figure 3.3-8. Linkage between the Secondary Engineered Barrier and the EDZ

3.3.2.4 Far Field

The far-field component of the current clay GDS model is shown schematically in Figure 3.3-9. This formulation consists of 20×20 node network of batch-reactor mixing cells used to represent 2D radionuclide transport. Releases from the near field enter the far field at the corner of the far-field cell network. Radionuclide transport is assumed to occur primarily via diffusive mechanisms. However, the model includes advective coupling between the mixing cells to evaluate sensitivity.

The following assumptions are inherent in this model.

- The “depth” of each mixing cell equals the “depth” of the unit cell within the model (i.e., distance between the centers of single waste packages in a horizontal emplacement conceptual design)
- Reflective boundary conditions at (1) the center of each emplacement drift/tunnel, (2) at the centerline between emplacement drifts/tunnels, and (3) at the plane of the emplacement drifts.
- Dissolved concentration limits are applied in each mixing cell.
- Reversible sorption in each mixing cell.

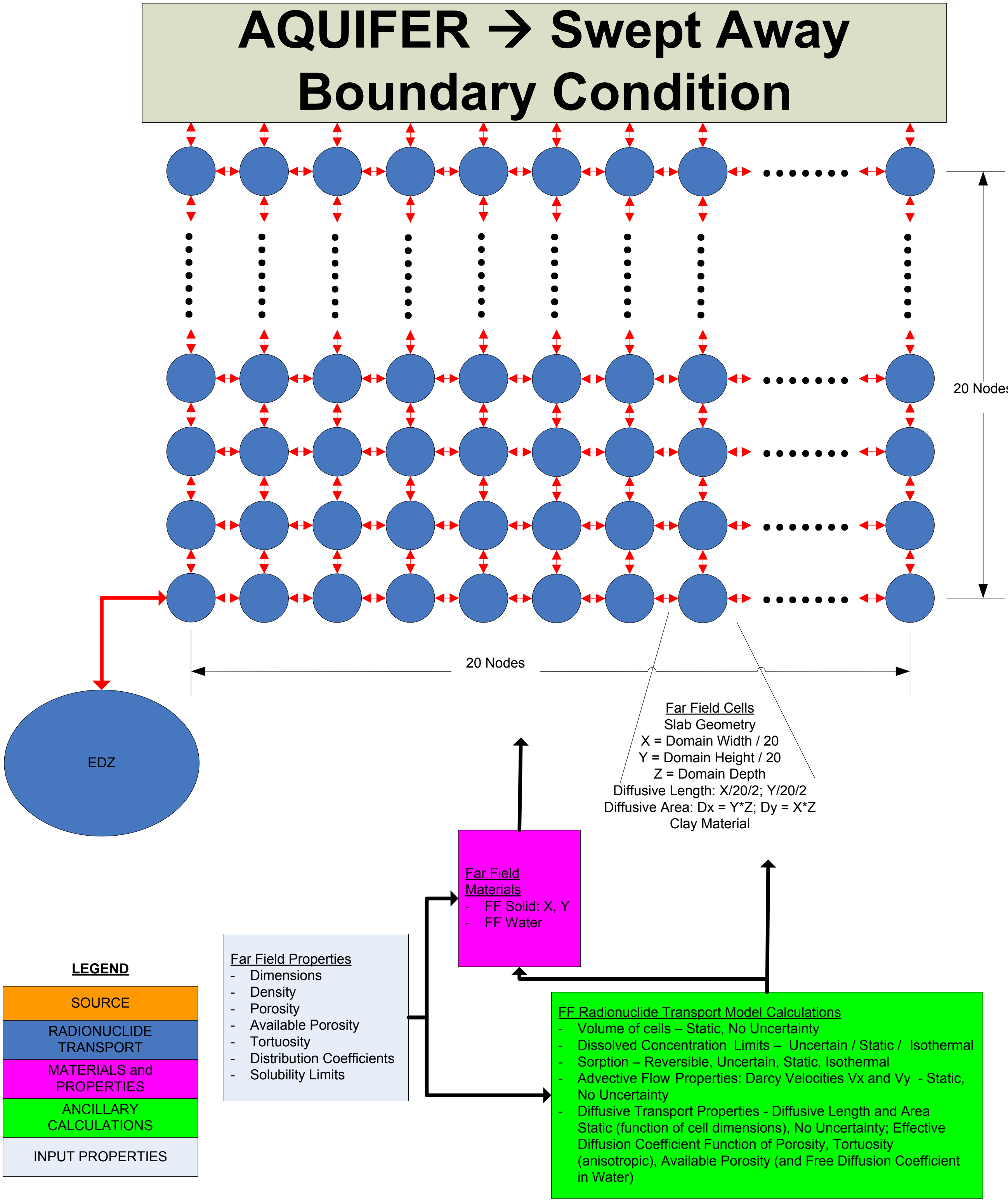
As discussed above (Figure 3.3-3), the far-field domain height, width, and depth are represented parametrically within the model and are defined by the user. Thus, the model is extremely flexible and can accommodate different repository configurations (e.g., spacing of emplaced waste). Thermal modeling and analysis tools could be used to determine allowable configurations for a prescribed waste form and conceptual repository design that would then be input into the clay GDS model.

The properties included in the far-field component of the clay GDS model are shown in Table 3.3-9. The porosity, density, and tortuosity of the far-field media are represented as triangular distributions with the minimum, most likely, and maximum values being input parameters. Different values for tortuosity can be defined in the horizontal and vertical directions to represent anisotropic diffusive radionuclide transport.

Table 3.3-9. Far-Field Properties

Property	Minimum	Most Likely	Maximum
Porosity	0.15	0.20	0.25
Density (kg/m^3)	2000	2250	2500
Tortuosity: X-dimension	0.5	0.75	0.1
Tortuosity: Y-dimension	0.25	0.5	0.75

NOTE: The values shown are for example only.



NOTE: The "swept-away" boundary condition for Aquifer refers to the assumption of a very large volumetric flow rate in the aquifer (to a sink), which effectively removes any radionuclides released from the clay far field.

Figure 3.3-9. Schematic of Far-Field Representation

The volume of each batch-reactor mixing cell is determined assuming each cell is a rectangular parallelepiped as:

$$V_{cell} = \frac{W_{domain}}{20} \bullet \frac{H_{domain}}{20} \bullet D_{domain} \qquad \text{Eq. 3.3-12}$$

where

V_{cell}	=	Volume of each cell in the 20x20 node grid (m^3)
W_{domain}	=	Width of the model domain (m); Figure 3.3-3
H_{domain}	=	Height of the model domain (m); Figure 3.3-3
D_{domain}	=	Depth of the model domain (m); Figure 3.3-3

The volume of water in each batch-reactor mixing cell is equal to the product of the cell volume and the porosity. The mass of solid material in the mixing cell is equal to the product of the volume of the cell and the density (assumed to be the dry density).

In the current model version, the ability to simulate dissolution/precipitation and reversible sorption is also included in each far-field batch reactor mixing cell in the same manner as was discussed above for the EBS and EDZ cells. Again, the model can be modified in the future should future investigations indicate that different probability distributions should be used or to involve explicit coupling to geochemical conditions and temperature within the batch reactor mixing cells.

Two-dimensional diffusion is modeled with the diffusive area and diffusive length in the horizontal and vertical directions determined as:

Diffusive Direction	**Diffusive Area**	**Diffusive Length**
Horizontal	$\frac{H_{domain}}{20} \bullet D_{domain}$	$\frac{W_{domain}}{20}$
Vertical	$\frac{W_{domain}}{20} \bullet D_{domain}$	$\frac{H_{domain}}{20}$

The effective diffusion coefficient is given as:

$$D_{eff,j} = D_{ref} \bullet R_{D,j} \bullet \phi \bullet \tau \bullet \phi_{A,j} \qquad \text{Eq. 3.3-13}$$

where

$D_{eff,j}$	=	Effective diffusion coefficient for element j (m^2/yr)
D_{ref}	=	Reference diffusivity in water (m^2/yr); Table 3.3-4
$R_{D,j}$	=	Relative diffusivity in water for element j; Table 3.3-4
ϕ	=	Porosity
τ	=	Tortuosity
$\phi_{A,j}$	=	Available porosity for element j (0 – 1); Table 3.3-7

This approach for determining the effective diffusion coefficient provides flexibility to the user in representing diffusive radionuclide transport in the far field. As discussed above, both the reference diffusivity and the element-specific relative diffusivities are user inputs. The element-specific available porosities are represented as triangular distributions with the minimum, most likely, and maximum values being user inputs as shown in Table 3.3-7. To represent anisotropic diffusive radionuclide transport, different values for the available porosity can be defined in the horizontal and vertical directions.

As discussed above, the far-field component of the current clay GDS model includes advective links between the batch-reactor cells in both the horizontal and vertical directions. Darcy velocities (V_x, V_z; m/yr) can be entered in both the vertical and horizontal directions. The volumetric flow rates are determined as:

Advective Direction	Volumetric Flow Rate (m^3/yr)
Horizontal	$V_x \bullet \frac{H_{domain}}{20} \bullet D_{domain}$
Vertical	$V_z \bullet \frac{W_{domain}}{20} \bullet D_{domain}$

3.3.2.5 Aquifer

The radionuclide concentration in the Aquifer in the clay GDS model is assumed to equal zero. This is accomplished by assuming a very large volumetric flow rate in the aquifer (to a sink), which effectively removes any radionuclides released from the clay far field. The radionuclide mass flux reaching the aquifer is used to determine the annual dose to the receptor. The mass flux for each radionuclide (g/yr) is multiplied by the specific activity (Bq/g) to determine the activity flux (Bq/yr) entering the aquifer.

3.3.2.6 Biosphere

The IAEA BIOMASS ERB1B dose model is used to convert the output radionuclide concentrations in the ground water at a hypothetical drinking well location to an estimate of annual dose based on drinking well water consumption (IAEA 2003). The biosphere model and parameter values for the clay GDS biosphere are the same as for the salt GDS biosphere (Section 3.1.2.8) and the granite GDS biosphere (Section 3.2.2.8).

3.3.2.7 Fast Paths

The current clay GDS model includes the capability to represent fast paths that can be parameterized by the user to evaluate various stylized scenarios.

The current far-field component of the clay GDS model, discussed above, includes the ability to include vertical advective transport within the far field at 25%, 50%, 75%, and 100% of the domain width within the 20×20 node network. This allows for the simulation of fast paths that do not directly intersect the emplaced waste or the engineered barriers, but could degrade the isolation capability of the far field. The user is able to define the Darcy velocity in these fast paths along with a time and duration that the increased flow occurs. The input parameters are shown in Table 3.3-10.

The current clay GDS model also includes the capability to evaluate stylized scenarios of preferential fast pathways that either directly intersect the emplaced waste or the engineered barriers. This capability is shown schematically in Figure 3.3-7. The model is comprised of a diffusive and an advective radionuclide transport component. The diffusive pathway consists of a five node network of batch-reactor mixing cells to represent 1D diffusion. This diffusive pathway is linked to a two segment "pipe" network that represent 1D advective-dispersive radionuclide transport between the diffusive network and the aquifer. A fast pathway scenario is defined by:

- Defining whether the fast-path network directly intersects the emplaced waste or other engineered barriers.
- Defining the distance for diffusive transport between the intersection point and the location where an advective fast-path is present;
- Defining the cross-sectional area for diffusive radionuclide transport (constant along the 1D direction)
- The length and advective (Darcy) velocity in each of the two advective-dispersive segments.

The properties of the fast path are shown in Table 3.3-11 and are applied to both the diffusive and advective segment. The ability to simulate dissolution/precipitation and reversible sorption is included in each batch-reactor mixing cell for the diffusive segment. Reversible sorption is included in each advective-dispersive "pipe." The dispersivity in each advective-dispersive "pipe" is assumed to be 10% of the segment length. It is assumed that the dissolved concentration limits and distribution coefficients are represented in the current clay GDS model as log-triangular, as shown in Table 3.3-4, with the user having the ability to define the minimum, best estimate, and maximum values of the distribution from the input spreadsheet for the fast pathway scenario.

Table 3.3-10. Far-Field Fast Path Parameters

Position in the Far-Field Domain	Velocity (m/yr)	Start Time (yr)	Duration (yr)
25%	6.31E-06	1.00E+06	2.00E+05
50%	0		
75%	0		
100%	0		

NOTE: The values shown are for example only.

Table 3.3-11. Fast Path Properties

Property	Minimum	Most Likely	Maximum
Porosity	0.15	0.20	0.25
Density (kg/m^3)	2000	2250	2500
Tortuosity	0.5	0.75	0.1

NOTE: The values shown are for example only.

The volume of each batch-reactor mixing cell is determined as:

$$V_{FP-Diffusion} = \frac{L_{FP-Diffusion}}{5} \bullet A_{FP-Diffusion} \quad \text{Eq. 3.3-14}$$

where

$V_{FP\text{-}Diffusion}$	=	Volume of each batch-reactor cell in the five-node diffusive network (m^3)
$L_{FP\text{-}Diffusion}$	=	Length of the five-node diffusive network (m); 5 cells along the length
$A_{FP\text{-}Diffusion}$	=	Cross-sectional area for diffusive radionuclide transport (m^2)

The volume of water in each batch-reactor mixing cell is equal to the product of the cell volume and the porosity. The mass of solid material in the mixing cell is equal to the product of the volume of the cell and the density (assumed to be the dry density).

The diffusive length in each cell is determined from the length of the five-node diffusive network (as $L_{FP\text{-}Diffusion}/5$).

As discussed above, the location where the preferential fast path intersects the EBS is either directly to the emplaced waste or to the secondary EBS. For the former, the entire inventory of waste is instantaneously released into the first diffusive batch-reactor mixing cell. If the latter is selected, the entire “base” model is executed to determine the release rate from the secondary barrier and that mass flux exiting is input into the first diffusive batch-reactor mixing cell. For both cases, all radionuclides are assumed to be transported through the preferential fast-pathway network. This neglects any additional radionuclide transport processes that would occur along the fast pathways (i.e., transverse diffusion into the far field) and will tend to overestimate release.

Two additional “fine” batch-reactor mixing cells are included before the five-node diffusive cell network. These cells are assumed to be 0.1-m thick and are included to better capture dissolution/precipitation processes for scenarios where the preferential fast pathway directly intersects the emplaced waste.

The effective diffusion coefficient is given as:

$$D_{eff,j} = D_{ref} \bullet R_{D,j} \bullet \phi \bullet \tau \bullet \phi_{A,j} \quad \text{Eq. 3.3-15}$$

where

$D_{eff,j}$	=	Effective diffusion coefficient for element j (m^2/yr)
D_{ref}	=	Reference diffusivity in water (m^2/yr); Table 3.3-4
$R_{D,j}$	=	Relative diffusivity in water for element j; Table 3.3-4
ϕ	=	Porosity
τ	=	Tortuosity
$\phi_{A,j}$	=	Available porosity for element j (0-1); Table 3.3-7

This approach for determining the effective diffusion coefficient provides flexibility to the user in representing diffusive radionuclide transport in the preferential fast-pathways. As discussed above, both the reference diffusivity and the element-specific relative diffusivities are user inputs. The element-specific available porosities are represented as triangular distributions with the minimum, most likely, and maximum values being user inputs as shown in Table 3.3-7.

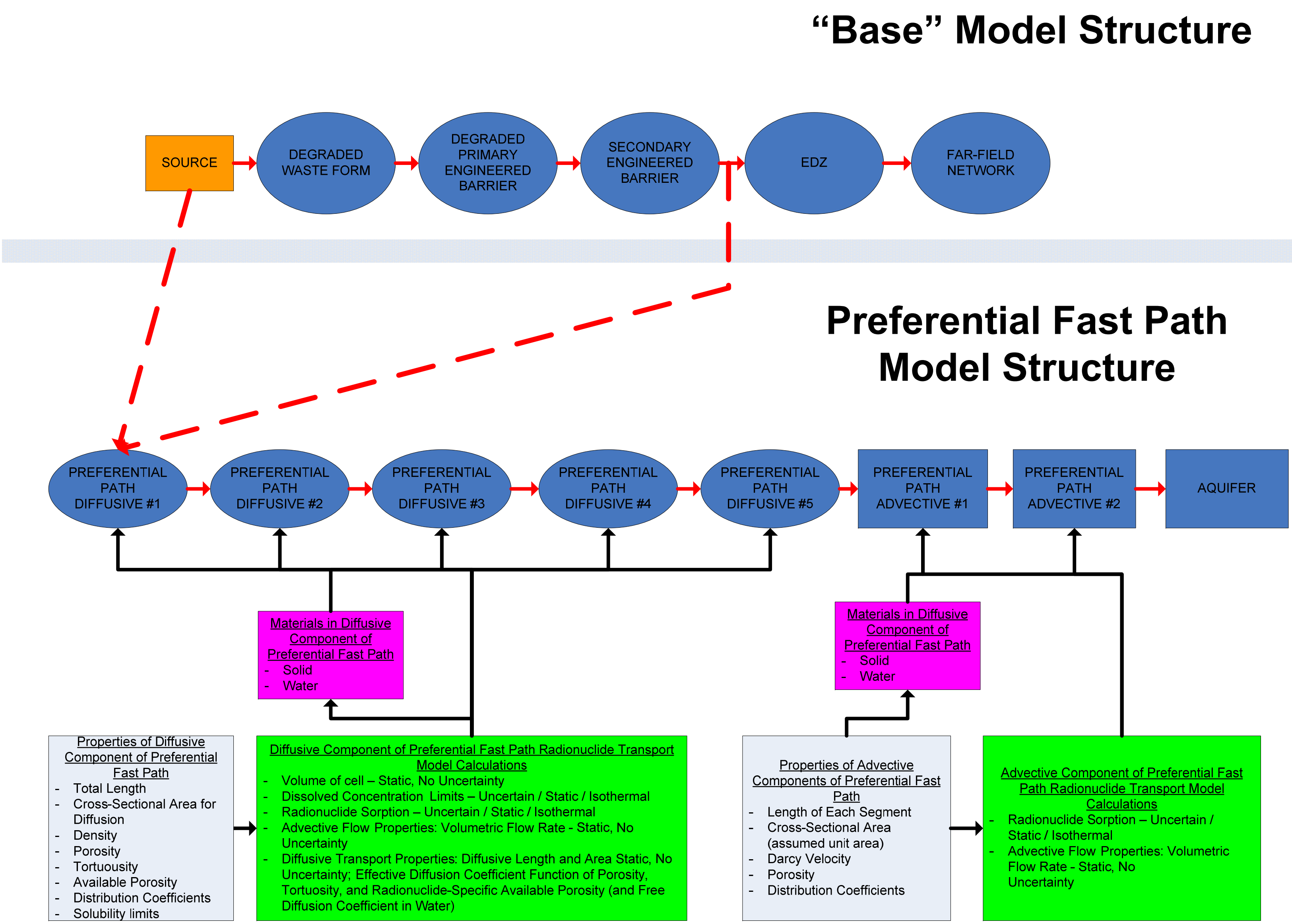


Figure 3.3-10. Schematic of Fast Pathway Simulation Capability

3.3.3 Confidence-Building Activities

This subsection discusses confidence-building activities that were performed with the current clay GDS model. The purpose of these activities were to build confidence in the results generated by the clay GDS model with regard to modeling generic clay disposal environments.

3.3.3.1 Far-Field Analytic Comparison

The ability of the numerical model to represent a wide range of dimensions was examined by comparing numerical and analytic solutions of the same diffusive transport problem. The comparisons indicate that as the aspect ratio of the numerical grid blocks making up the far field becomes larger, agreement between the numerical solution produced by GoldSim and the exact analytic solution deteriorates. However, even with the rather extreme ratio of 15/2, disagreement seems at worst to be only about 10% at only a few limited locations, primarily in the corners closest to and farthest away from the interface with the near field/EDZ.

In the absence of advective flow the 20 × 20 matrix of cells used to represent the far field solves a time-dependent diffusion equation in two spatial dimensions. For species that are not limited by solubility and not undergoing radioactive decay, in an isotropic medium this equation is

$$\frac{\partial c}{\partial t} = D\left[\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right], \qquad \text{Eq. 3.3-16}$$

where t is the time, $0 \le x \le a$ and $0 \le y \le b$ with a the width of the far field and b the depth, D is the bulk diffusion coefficient (see Equations 4-6 though 4-9 for further details), and c is the concentration. Using the technique of separation of variables and applying the initial and boundary conditions

$$c(0,x,y) = \frac{M}{\delta\varepsilon} \text{ when } (0 \le x \le \delta), (0 \le y \le \varepsilon) \text{ and } = 0, \text{ otherwise},$$

$$D\left.\frac{\partial c}{\partial x}\right|_{x=0} = D\left.\frac{\partial c}{\partial x}\right|_{x=a} = 0 \qquad \text{Eq. 3.3-17}$$

at all times t and positions y, and

$$c(t,x,b) = D\left.\frac{\partial c}{\partial y}\right|_{y=0} = 0 \qquad \text{Eq. 3.3-18}$$

for all values of t and x, the solution for this equation is found to be

$$c(t,x,y) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} A_{nm} e^{-k_{nm} t} \cos(\alpha_n x)\cos(\beta_m y). \qquad \text{Eq. 3.3-19}$$

In the foregoing equations, M is the mass (per unit length in a direction perpendicular to the x,y plane) initially confined to the area $(0 \le x \le \delta)$, $(0 \le y \le \varepsilon)$,

$$\alpha_n = \frac{n\pi}{a},$$

$$\beta_m = \frac{(2m+1)\pi}{2b},$$

and

$$k_{nm} = D\left(\alpha_n^2 + \beta_m^2\right).$$

When $n = 0$,

$$A_{0m} = \frac{2M}{ab\varepsilon\beta_m}\sin(\beta_m\varepsilon),$$

and when $n > 0$,

$$A_{nm} = \frac{4M}{ab\delta\varepsilon\alpha_n\beta_m}\sin(\alpha_n\delta)\sin(\beta_m\varepsilon).$$

Except when t is near zero, a relatively small number of terms provides adequate convergence for the series in Equation 3.3-19.

To provide an indication of the robustness of the GoldSim solution in the clay GDS model when the 20 × 20 matrix cells represent a variety of sizes and aspect ratios for the rectangular far-field region, the numerical GoldSim solution was compared with the exact solution as given by Equation 3.3-19. For this purpose, 10 grams of a test species was inserted at time zero into the GoldSim cell representing the part of the region defined by $(0 \le x \le \delta)$, $(0 \le y \le \varepsilon)$ where $\delta = a/20$ and $\varepsilon = b/20$. This region has a thickness perpendicular to the x,y plane of 1.6 m. In the graphs that follow, the cell where the mass is inserted has the label X1Y1, a cell approximately in the middle of the rectangular region has the label X10Y10, and the cell at the opposite corner of the region from the cell X1Y1 has the label X20Y20. A point at the center of the cell X1Y1 has the coordinates $x = \delta/2$ and $y = \varepsilon/2$, a point at the center of the cell X10Y10 has the coordinates $x = 9.5\delta$ and $y = 9.5\varepsilon$, and a point at the center of the cell X20Y20 has coordinates $x = 19.5\delta$ and $y = 19.5\varepsilon$. The bulk diffusion coefficient has the value 2×10^{-10} m^2/s.

For the first set of comparisons, a square far field with a width $a = 20$ m and a depth $b = 20$ m is considered. The time-dependent concentration in the three cells referred to in the foregoing paragraph is shown in Figure 3.3-11. Comparisons between the two solutions were also made at several other locations within the matrix with agreement as good as shown for X10Y10 and X20Y20. Agreement is not as good for X1Y1 because the spatial mesh is not sufficient for tracking the step-function behavior of the concentration at early times. Calculations were also completed for square far fields with dimensions as large as $a = b = 80$ m with the same quality of agreement as shown in Figure 3.3-11. The only effect of changing the size of the square far field is to change the time constants k_{nm} in Equation 3.3-19.

Results for a second set of calculations for a rectangular far field with $a = 20$ m and $b = 80$ m. Comparisons between the GoldSim numerical solution and the exact solution from Equation 3.3-19 are shown in Figure 3.3-12. While agreement is not quite as good as is shown in Figure 3.3-11, the GoldSim numerical result is, nevertheless, within a few percent of the exact solution except in the cell X1Y1. As in the previous case, results were compared at several additional locations within the far field and in all cases agreement was as good as or better than shown in Figure 3.3-12.

A third set of calculations were carried out for a rectangular far field with $a = 80$ m and $b = 20$ m. Comparisons for this case are shown in Figure 3.3-13. This case differs from that shown in Figure 3.3-12 in that leakage occurs along the long side of the rectangle rather than the short side. Agreement between the numerical and exact solutions is slightly worse in this case than in the case shown in Figure 3.3-12, but even so, the most serious disagreement is only about 4% except in the case of the cell X1Y1.

The fourth set of calculations involved the more extreme aspect ratio in which the rectangular far field has $a = 20$ m and $b = 150$ m. Results for this case are shown in Figure 3.3-14. Agreement is very good in the cell near the center of the far field but GoldSim over-predicts the concentration by slightly more than 10% at the corner of the rectangle opposite where the mass in inserted. There are other locations in the far field where the disagreement between GoldSim's numerical solution and the exact solution is similar to that shown in Figure 3.3-14 for the cell X20Y20. It is worth noting that even though the magnitude of the concentration is off, GoldSim seems to make an accurate prediction of the time when the peak concentration occurs.

Comparisons shown in Figures 3.3-11 through 3.3-14 indicate that as the aspect ratio becomes larger, agreement between the numerical solution produced by GoldSim and the exact solution given by Equation 3.3-19 deteriorates. However, even with the rather extreme ratio of 15/2, disagreement seems at worst to be only about 10%, at only a few limited locations, primarily in the corners closest to and farthest away from where the source was injected. Inserting mass into a single cell at time zero probably offers a more serious challenge to the numerical solution algorithm than the gradual release of mass into this cell over a longer period of time such as occurs in the repository analysis considered in this subsection. The difficulty could be avoided if it were possible to easily change the number of cells in the x and y directions and thus keep the ratio of the length to width of individual cells close to unity. However, this is not easily accommodated within the GoldSim software.

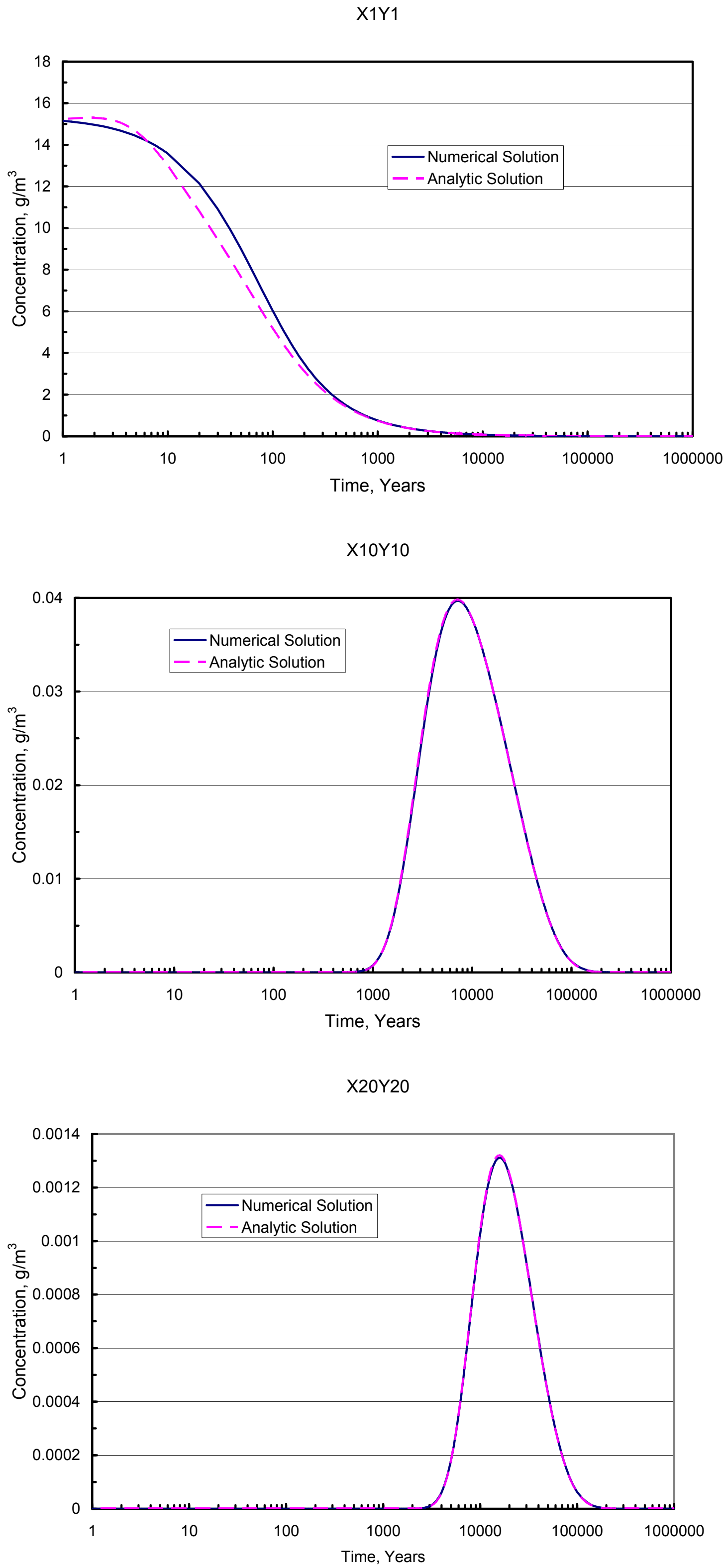


Figure 3.3-11. Time-Dependent Solutions for $a = 20\,\text{m}$ $b = 20\,\text{m}$

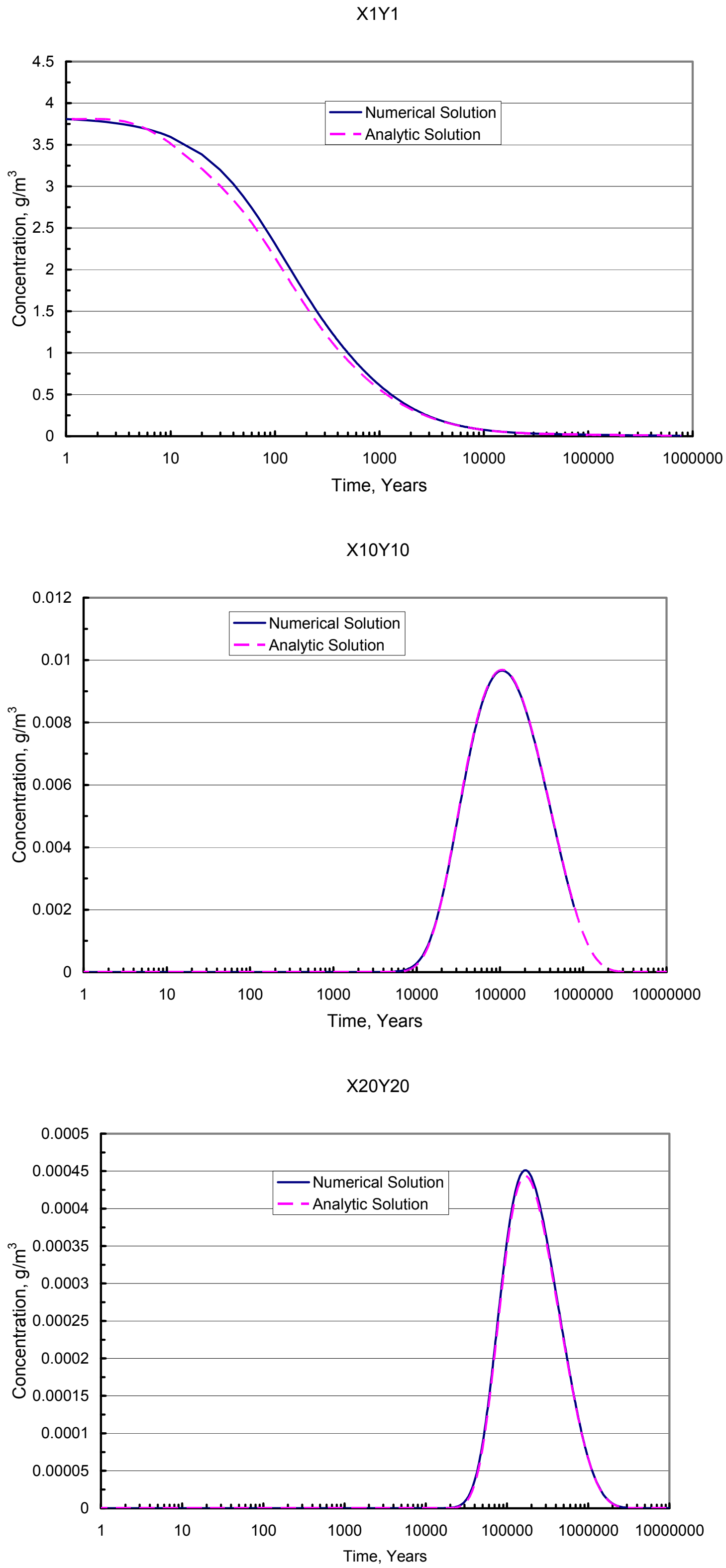


Figure 3.3-12. Time-Dependent Solutions for $a = 20\,\text{m}$ $b = 80\,\text{m}$

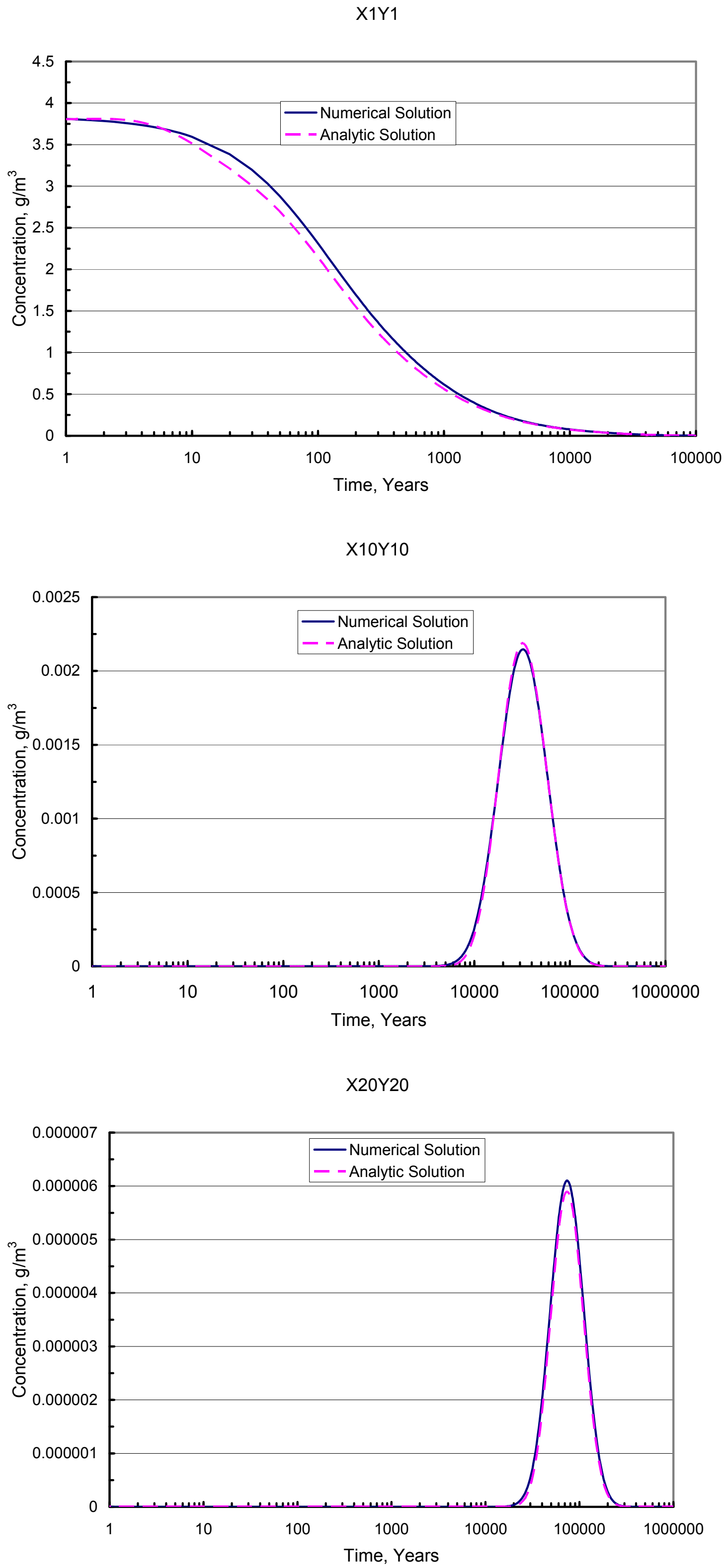


Figure 3.3-13. Time-Dependent Solutions for $a = 80\text{ m}$ $b = 20\text{ m}$

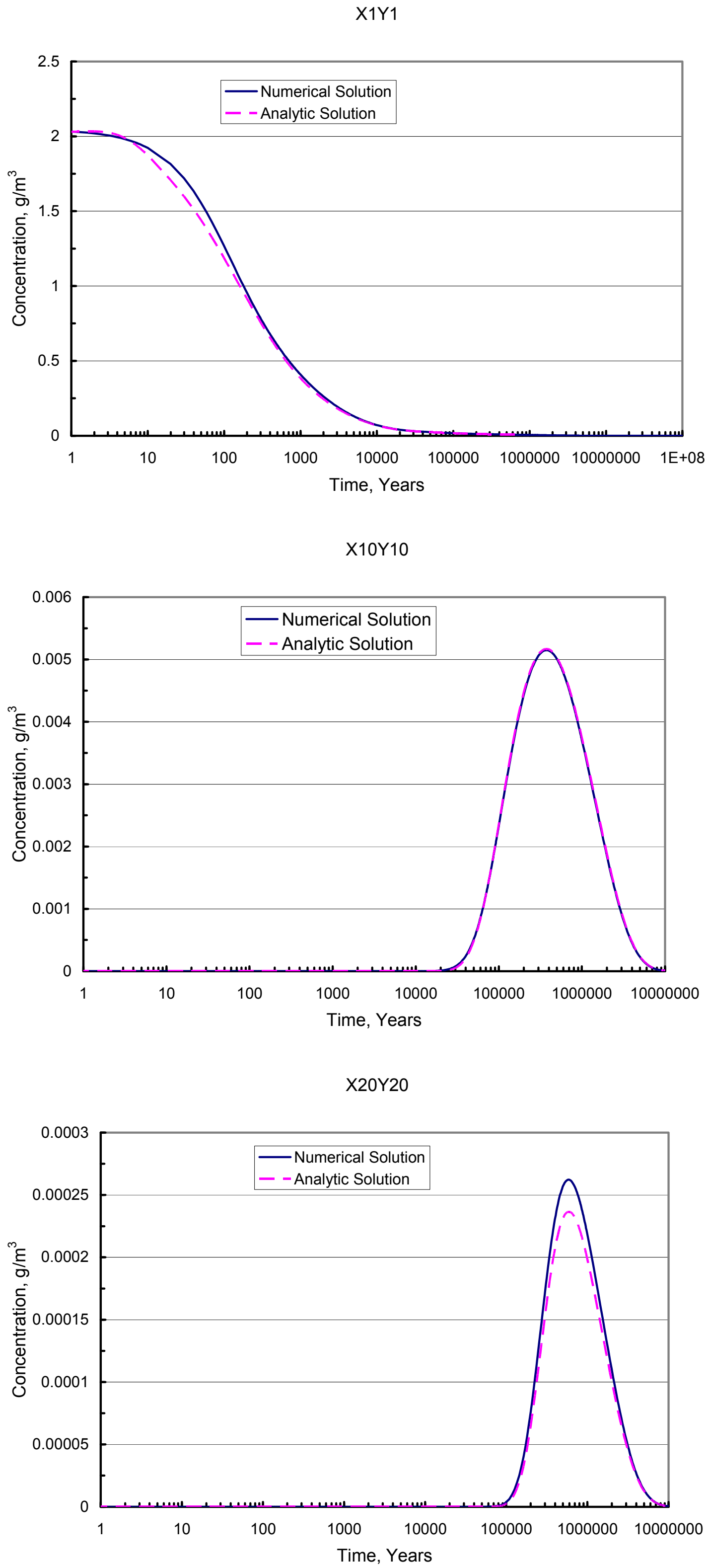


Figure 3.3-14. Time-Dependent Solutions for $a = 20\,\text{m}$ $b = 150\,\text{m}$

3.3.3.2 PAMINA Benchmark

3.3.3.2.1 Purpose of Analysis

The European Commission Performance Assessment Methodologies IN Application (PAMINA) to Guide the Development of the Safety Case project brought together 25 organizations from ten European countries and one European Community Joint Research Centre in order to improve and harmonize methodologies and tools for demonstrating the safety of deep geological disposal of long-lived radioactive waste for different waste types, repository designs and geological environments. One of the PAMINA tasks was to conduct several benchmark exercises on specific processes, in which quantitative comparisons were made between approaches that rely on simplifying assumptions and models, and those that rely on complex models that take into account a more complete process conceptualization in space and time. Benchmark calculations were performed and compared for clay, salt, and crystalline geologic disposal environments.

The current clay GDS model was used to perform the same benchmark calculations that were performed under the PAMINA project for clay disposal environments (Andra 2005a; Andra 2005b). The benchmark cases, repository configuration, radionuclide inventory, and parameters can be found in the PAMINA reports (Andra 2005a; Andra 2005b). Transport through the clay far field was modeled as occurring both via radionuclide diffusion and advection.

3.3.3.2.2 Model Description

Six radionuclides were included in the PAMINA clay benchmark to evaluate different radionuclide transport processes:

- *^{129}I*—Highly soluble and because it migrates as an anion, it does not adsorb on the negatively charged clay particles and is thus fairly mobile.
- *^{135}Cs*—Highly soluble with very strong sorption on the clay particles.
- *^{79}Se*—Migrates as an unretarded species and its release was assumed to be controlled by its solubility limit.
- *^{237}Np, ^{233}U, ^{229}Th*—In this benchmark, the 4N+1 actinide chain transport was limited to the following 3 members: $^{237}Np \rightarrow {}^{233}U \rightarrow {}^{229}Th$. These radionuclides are both solubility limited and strongly sorbing in the clay environment.

The disposal cell configuration considered in the PAMINA benchmark is shown in Figure 3.3-15 (Genty, Mathieu, and Weetjens 2009) and the parameters for this configuration are shown in Table 3.3-12 (Genty, Mathieu, and Weetjens 2009). This benchmark was executed with the clay GDS model using only the far-field component. The waste form, primary engineered barrier, secondary engineered barrier, and the EDZ components of the clay GDS model were not used (batch-reactor cell volumes set to 10^{-5} m^3, advective flow rates set to 10^{10} m^3/yr, dissolved concentration limits set to 10^{10} kg/m^3, and distribution coefficients set to 0 m^3/kg).

In the clay GDS model representation a domain width of 10 m and a domain depth of 30 m were used. These correspond to parameters L_d and L_w in Table 3.3-13. The domain height for Cs, I, and Se was 50 m, equal to half of the domain height considered in the PAMINA benchmark (parameter H_{hr} in Table 3.3-13). For Np, U, and Th, (4N+1 actinide chain) the PAMINA benchmark also considered a reduced thickness of the clay layer from 100 m to 40 m (parameter H_{hr} in Table 3.3-13) (Weetjens 2008). Thus, additional calculations were performed with the clay GDS model considering a reduced domain height of 20 m for Np, U, and Th.

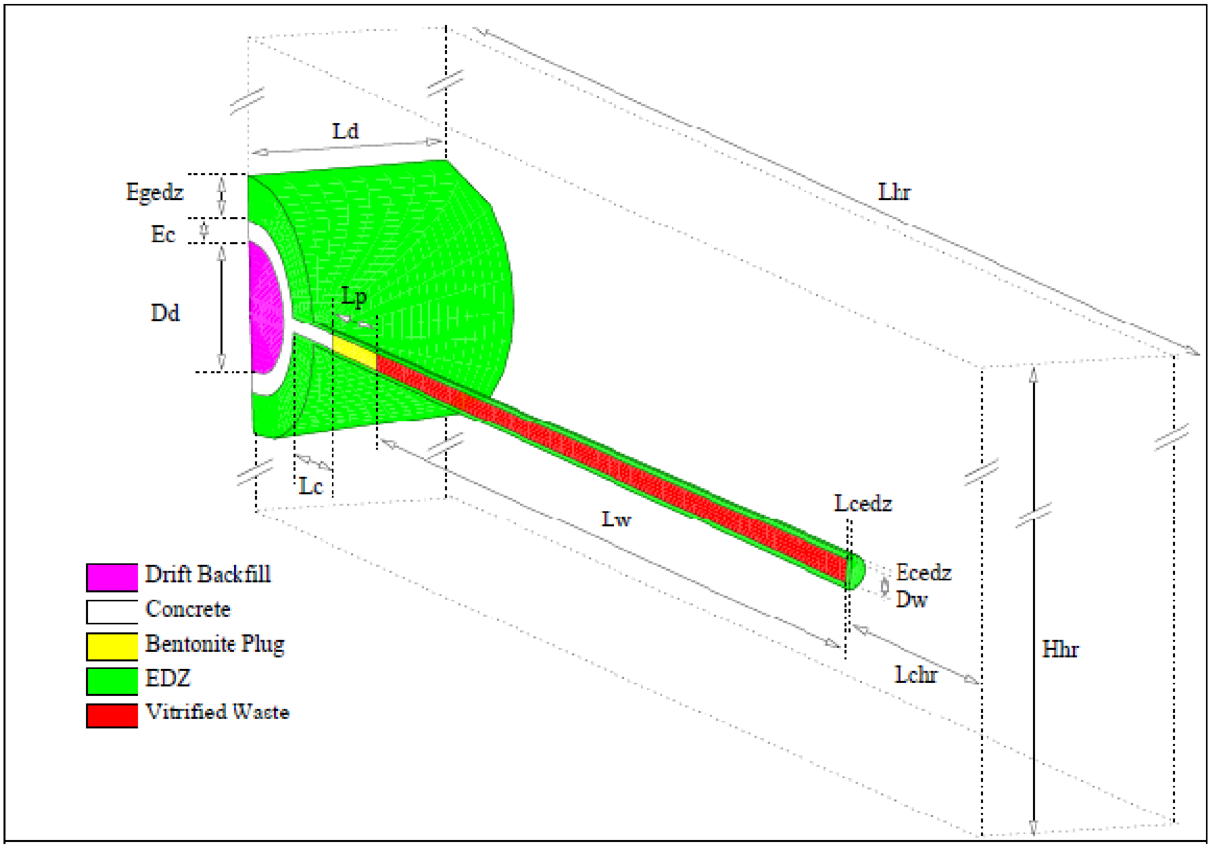


Figure 3.3-15. PAMINA Benchmark Configuration

Table 3.3-12. PAMINA Benchmark Configuration Parameters

Name	Description	Value (m)
Dd	Inner drift diameter	6
Ec	Concrete drift extension	1
Egedz	Drift EDZ extension	2
Ld	Drift length	10
Hhr	Host rock vertical extension	100
Lc	Concrete plug length	4
Lp	Bentonite plug length	4
Lw	Waste disposal cell length	30
Lcedz	Length of the EDZ at the end of the disposal cell	0.175
Lchr	Extension of host rock at the end of the disposal cell	10
Dw	Waste disposal cell diameter	0.70
Ecedz	EDZ extension around waste disposal cell	0.175
Lhr	Total Length of the calculation domain	52.175

The PAMINA benchmark assumed a vertical hydraulic conductivity of 10^{-13} m/s. Hydraulic heads were assumed to be 450 m at the bottom of the model domain and 350 m at the top of the model domain. These heads were used for both the 100-m and 40-m clay thickness cases for the 4N+1 actinide decay chain calculations. This resulted in Darcy velocities of 3.15×10^{-6} m/yr for the 100-m thickness and 7.88×10^{-6} m/yr for the 40-m thickness.

The far-field media properties are shown in Table 3.3-13. Note that the PAMINA benchmark calculations were deterministic. The properties for each radionuclide considered are shown in Table 3.3-14.

The PAMINA benchmark calculations (Andra 2005a; Andra 2005b) assumed a 4,000-yr waste package lifetime. However, the calculations performed using the clay GDS model assumed immediate failure of the waste package. This has an insignificant effect on the results, as shown below, due to the very long time periods for the peak radionuclide flux to occur (several hundred thousand to millions of years). The PAMINA benchmark calculations assumed a fractional waste form degradation rate of 10^{-5} yr^{-1}, which was also assumed in the clay GDS model calculations.

Table 3.3-13. Far-Field Properties – PAMINA Benchmark

Property	Value
Porosity	0.06
Density (kg/m^3)	2000
Tortuosity : X-dimension	0.01
Tortuosity : Y-dimension	0.01

Source: Genty, Mathieu, and Weetjens 2009, Table 6 (except for the density, which was assumed).

Table 3.3-14. Radionuclide Properties – PAMINA Benchmark

Radionuclide	Dissolved Concentration Limit (mol/L)[a]	Retardation Coefficient[b]	Distribution Coefficient (m^3/kg)[c]	Effective Diffusion Coefficient ($\times10^{-13}$ m^2/s)[d]	Available Porosity[e]
^{129}I	Soluble	Nonsorbing	Nonsorbing	6.48	0.47
^{135}Cs	Soluble	20	5.7×10^{-4}	4.32	0.31
^{79}Se	4.68×10^{-9}	Nonsorbing	Nonsorbing	6.78	0.49
^{237}Np	1.0×10^{-6}	10	2.7×10^{-4}	6.48	0.47
^{233}U	3.2×10^{-8}	3	6.0×10^{-5}	6.48	0.47
^{229}Th	5.0×10^{-7}	5	1.2×10^{-4}	6.48	0.47

NOTE: [a]From Genty, Mathieu, and Weetjens 2009, Table 6

[b] ^{137}Cs from Genty, Mathieu, and Weetjens 2009, Table 7; ^{237}Np, ^{233}U, ^{229}Th from Andra 2005b (the PAMINA benchmark calculations used a factor of 100 reduction in the retardation coefficients for these radionuclides below that reported in Andra 2005a, Table 7.)

[c]Calculated from $R=1+\rho K_d/\phi$; density (ρ) and porosity (ϕ) from Table 3.3-13

[d]From Genty, Mathieu, and Weetjens 2009, Table 8

[e]The available porosity was calculated using Equation 3.3-13 to yield the effective diffusive coefficient shown for a free diffusion coefficient of 2.3×10^{-9} m^2/s, radionuclide-specific relative diffusivities of 1, porosity from Table 3.3-13, and tortuosity from Table 3.3-13.

3.3.3.2.3 Analysis Results

The results from the clay GDS model are shown in Figure 3.3-16. The results shown are the activity flux entering the upper aquifer – the metric computed in the PAMINA benchmark calculations. Individual radionuclide comparisons are shown and discussed below. It must be recognized that the PAMINA benchmark allowed for both upward and downward vertical diffusion while the clay GDS model assumes all radionuclides diffuse upward. This difference alone would result in the clay GDS model over-estimating the resultant mass flux reaching the overlying aquifer by a factor of approximately two.

Overall, the comparisons of the clay GDS model and PAMINA benchmark results are excellent. This further indicates that the simplified representation of radionuclide transport in the clay GDS model is sufficient for the purposes of a generic simulation modeling tool of geologic disposal systems in clay.

^{129}I—A comparison between the clay GDS model and the PAMINA benchmark results is shown in Figure 3.3-17. It can be seen that the resultant activity flux to a hypothetical upper aquifer are similar, both in the magnitude of the flux and the timing of the breakthrough. The peak activity flux calculated with the clay GDS model occurs approximately 200,000 yr earlier than the results shown for the PAMINA benchmark. The magnitude of the peak activity is approximately a factor of 1.5 – 3 larger than the PAMINA benchmark results (direct comparison).

^{135}Cs—A comparison between the clay GDS model and the PAMINA benchmark results is shown in Figure 3.3-18. It can be seen that the resultant activity flux to a hypothetical upper aquifer are similar. The clay GDS model results in earlier breakthrough (~200,000 yr) and a factor of approximately 6 – 10 higher peak activity flux (direct comparison).

^{79}Se—^{79}Se migrates as an unretarded species and its release was assumed to be controlled by its solubility limit (4.68×10^{-9} mol/L). A comparison between the clay GDS model and the PAMINA benchmark results shows similar behavior (Figure 3.3-19). It can be seen that the resultant activity flux to a hypothetical upper aquifer are similar. The clay GDS model results in slightly delayed breakthrough and a factor of approximately 2 lower peak activity flux when compared to the majority of the PAMINA benchmark results (direct comparison).

4N+1 Chain—Comparison between the clay GDS model and the PAMINA benchmark results are shown in Figures 3.3-20 to 3.3-22 for the 4N+1 chain. Results are shown for the 100-m domain height case, for comparison with the PAMINA benchmark results from Institute of Radioprotection and Nuclear Safety and for the 40-m domain height case, for comparison with the results from SCK•CEN. It can be seen that the resultant activity flux to a hypothetical upper aquifer calculated by the clay GDS model are similar to the PAMINA benchmark for both domain height cases. The clay GDS model results in slightly delayed breakthrough and a factor of approximately 2 – 5 lower peak activity flux for the both the 40-m and 100-m domain cases (direct comparison).

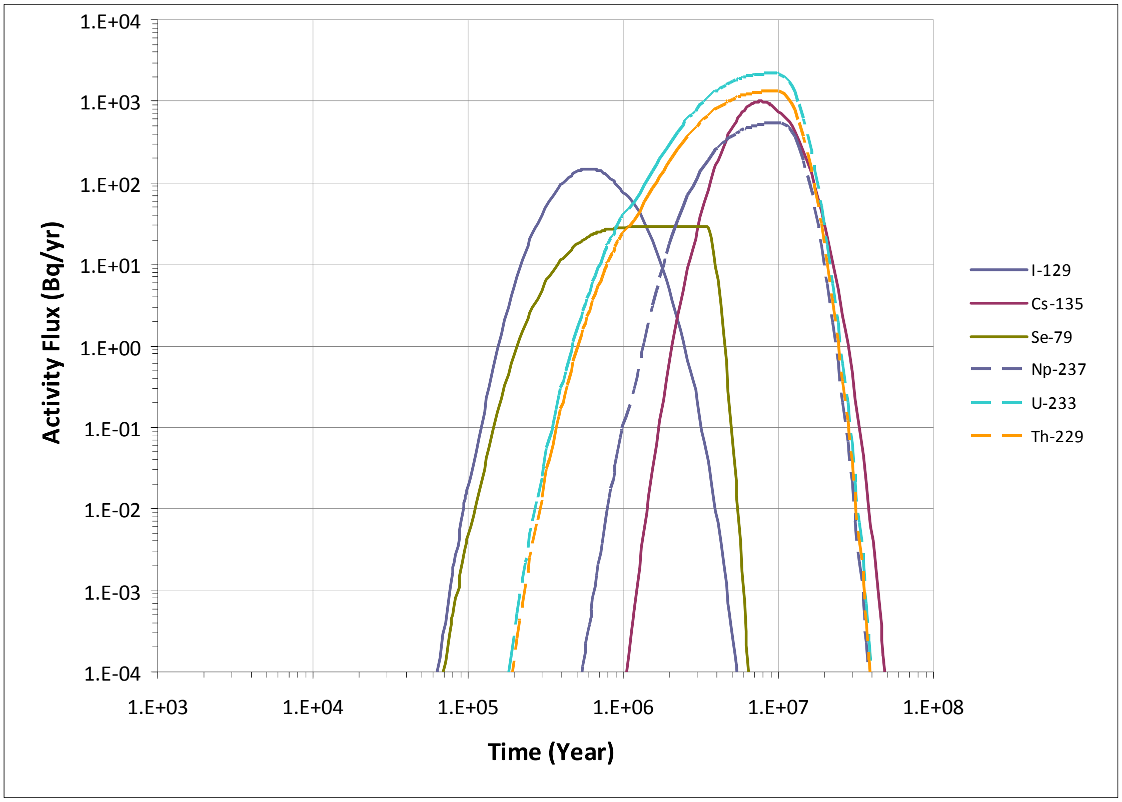
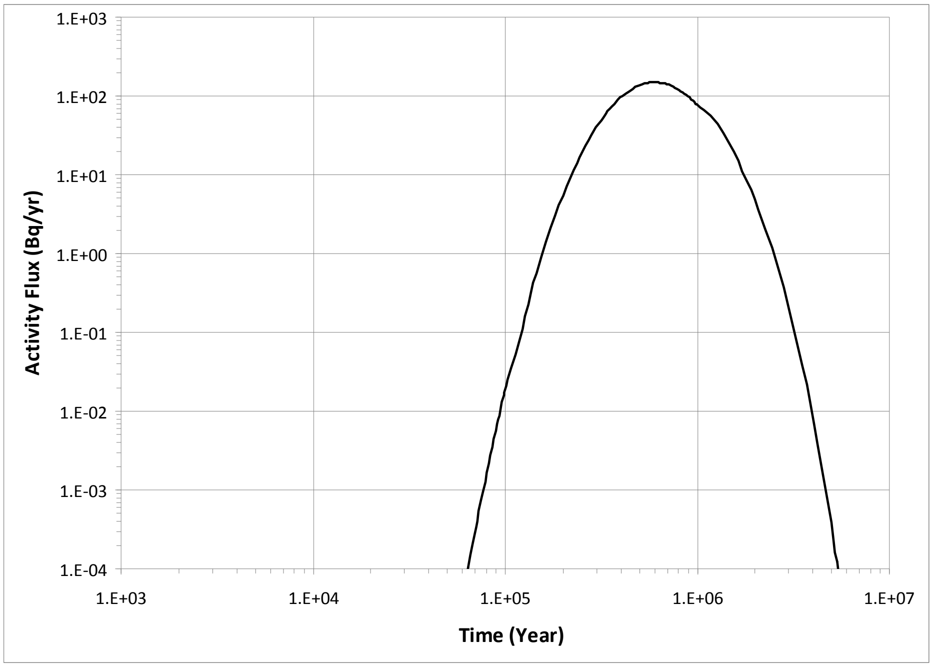
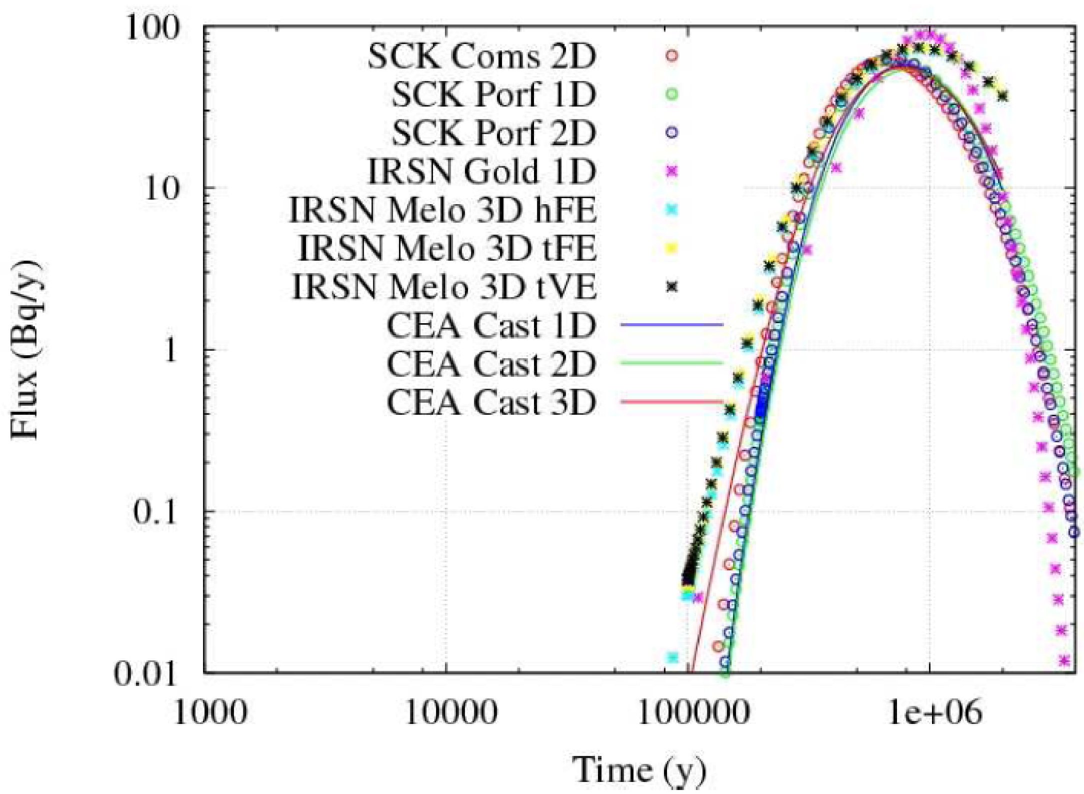


Figure 3.3-16. PAMINA Clay Benchmark Results using the Clay GDS Model

(a) Clay GDS Model



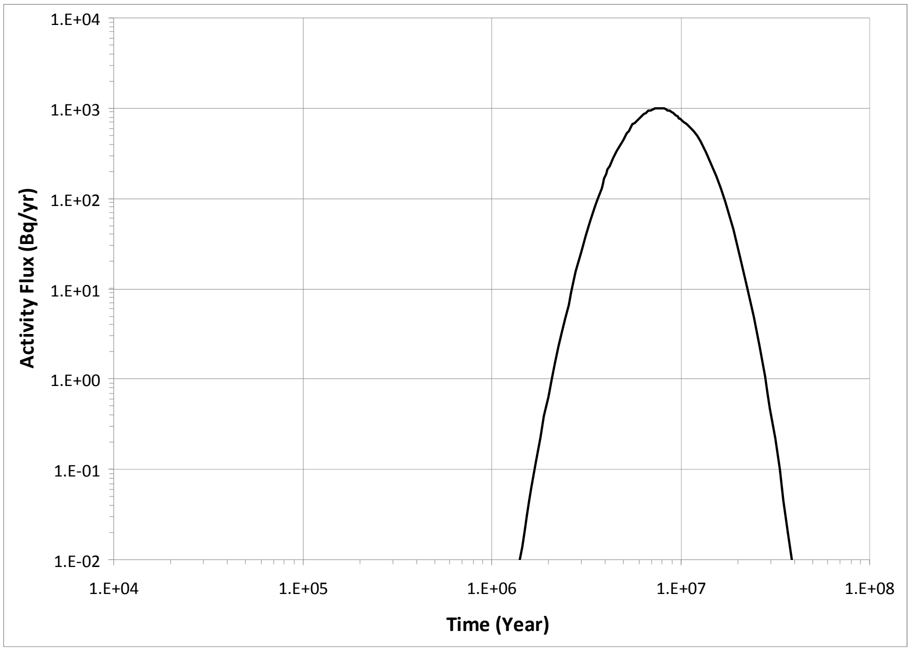
(b) PAMINA Benchmark



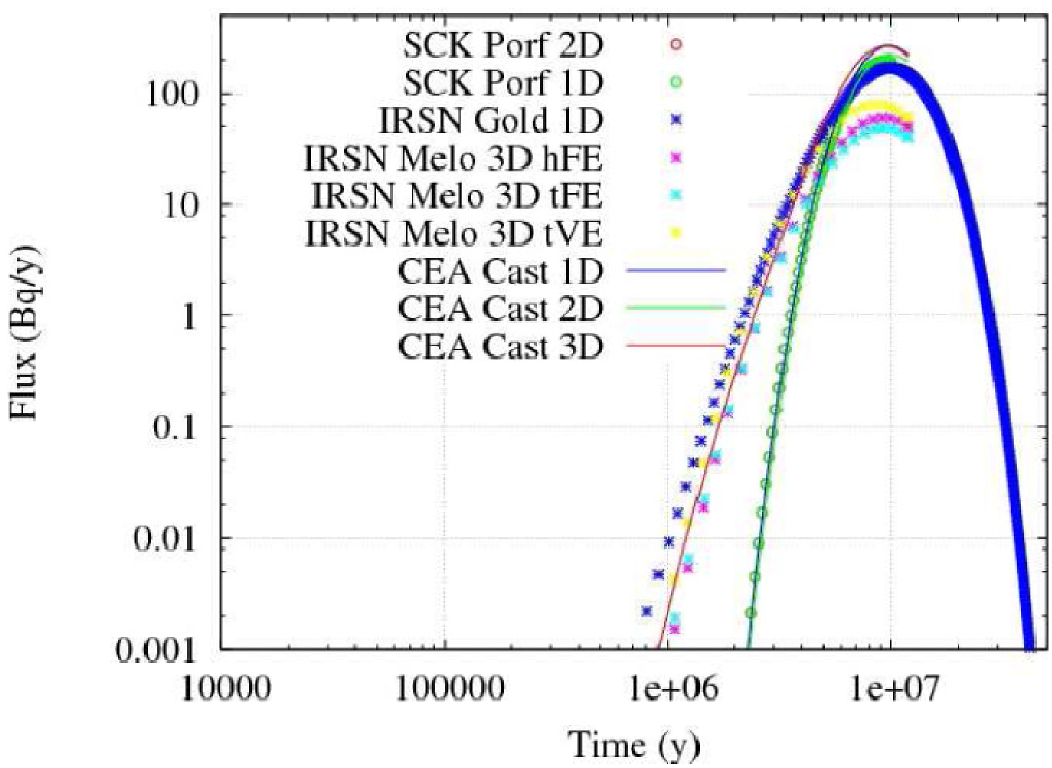
Source: Genty, Mathieu, and Weetjens 2009, Figure 13.

Figure 3.3-17. Iodine Activity Flux to Upper Aquifer– PAMINA Benchmark

(a) Clay GDS Model



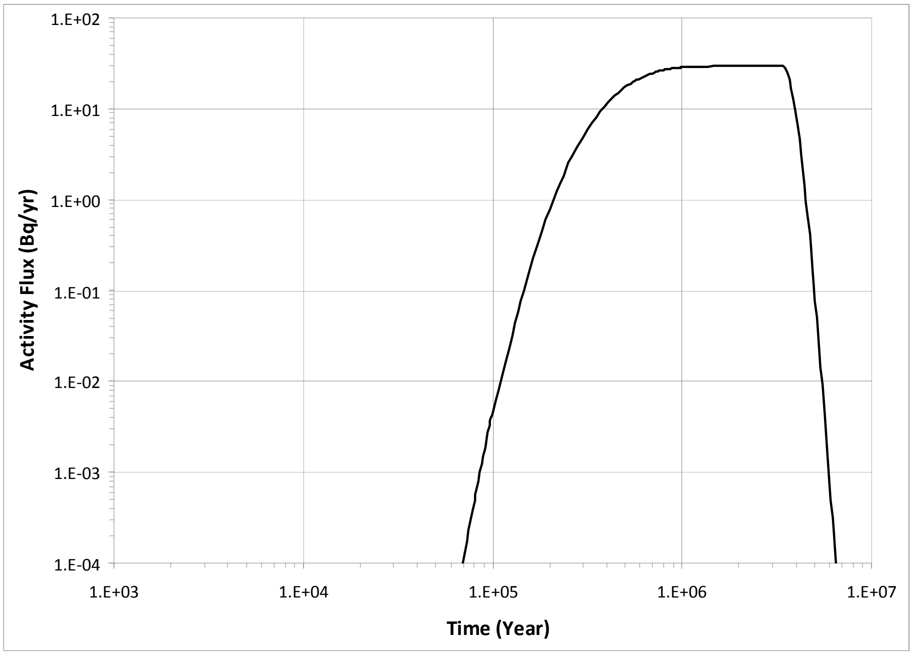
(b) PAMINA Benchmark



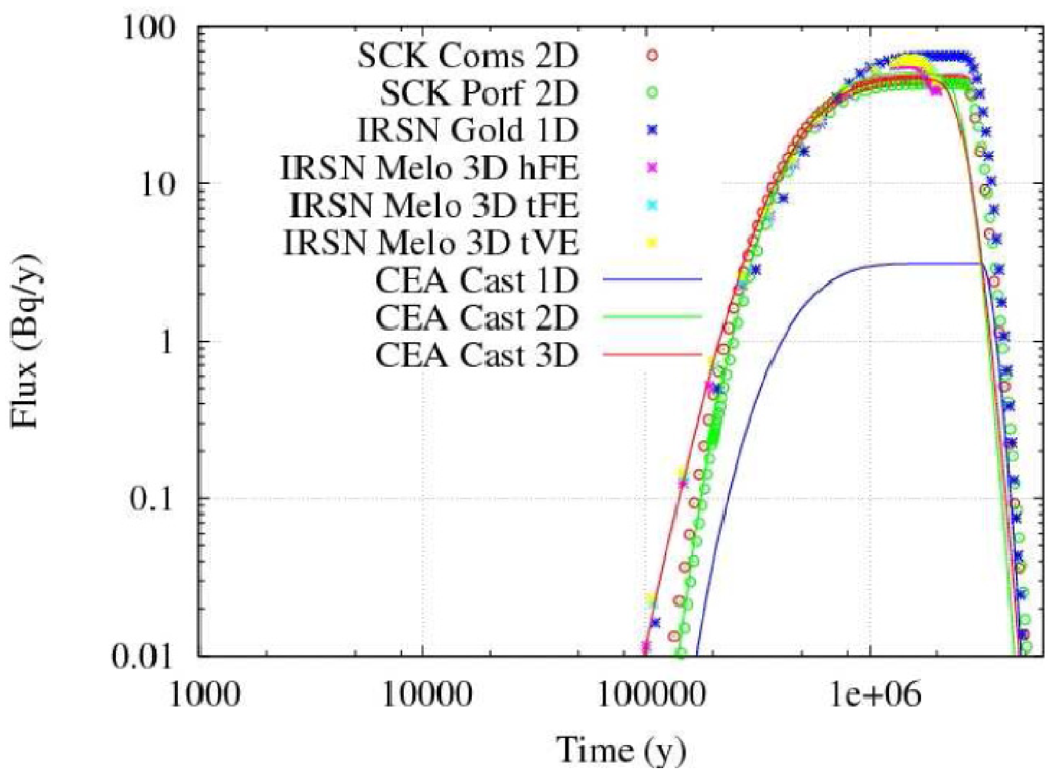
Source: Genty, Mathieu, and Weetjens 2009, Figure 14.

Figure 3.3-18. Cs Activity Flux to Upper Aquifer– PAMINA Benchmark

(a) Clay GDS Model



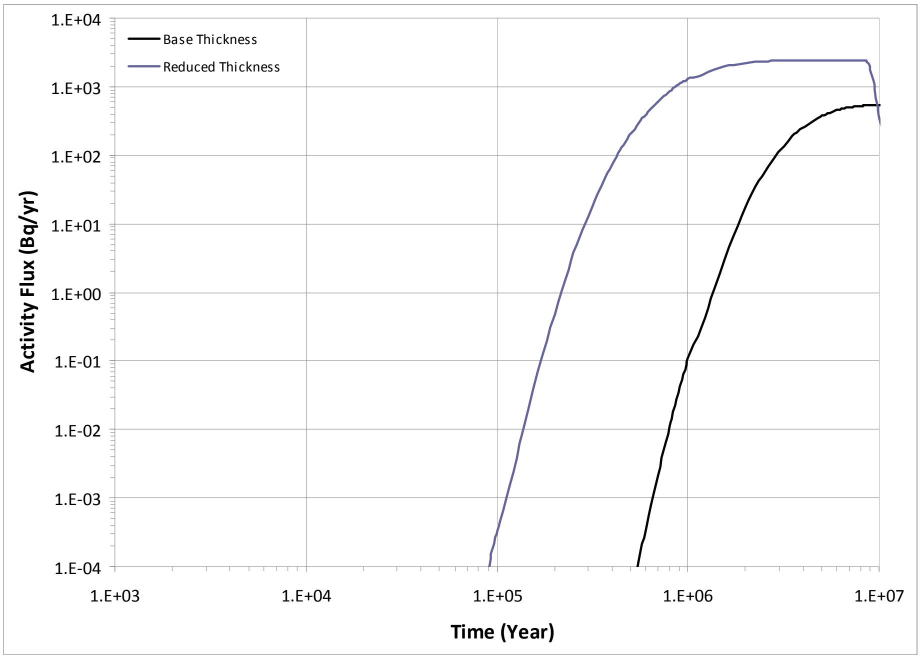
(b) PAMINA Benchmark



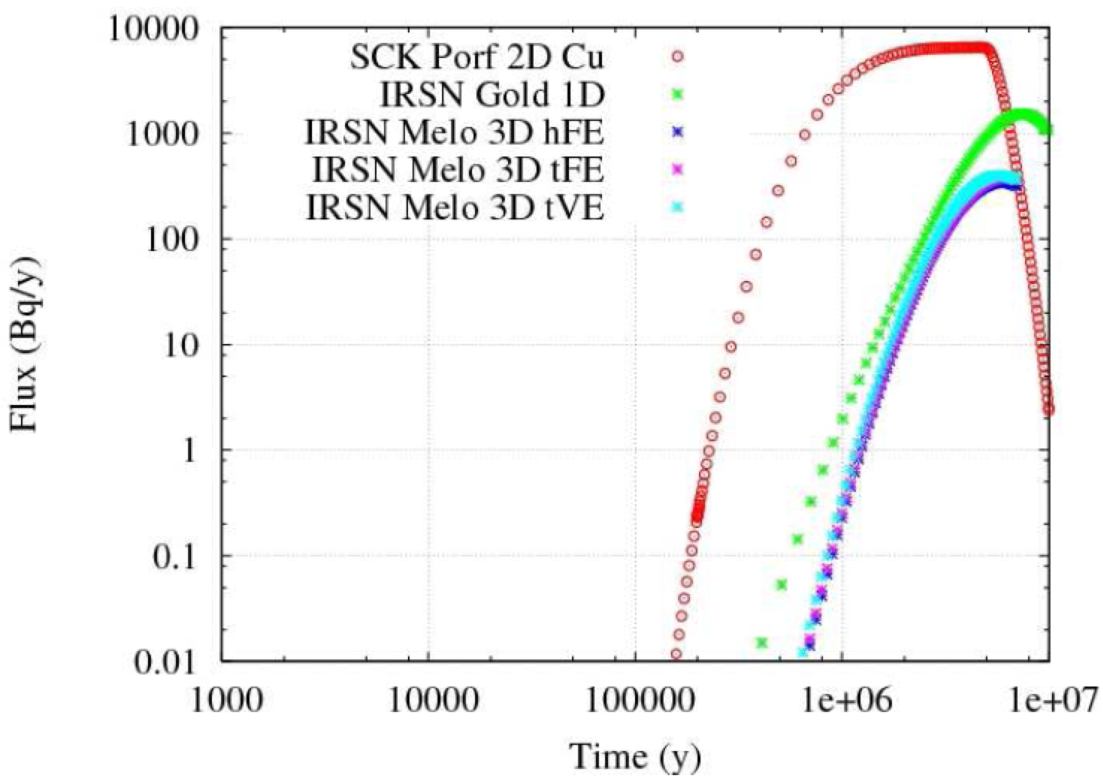
Source: Genty, Mathieu, and Weetjens 2009.

Figure 3.3-19. Se Activity Flux to Upper Aquifer– PAMINA Benchmark

(a) Clay GDS Model



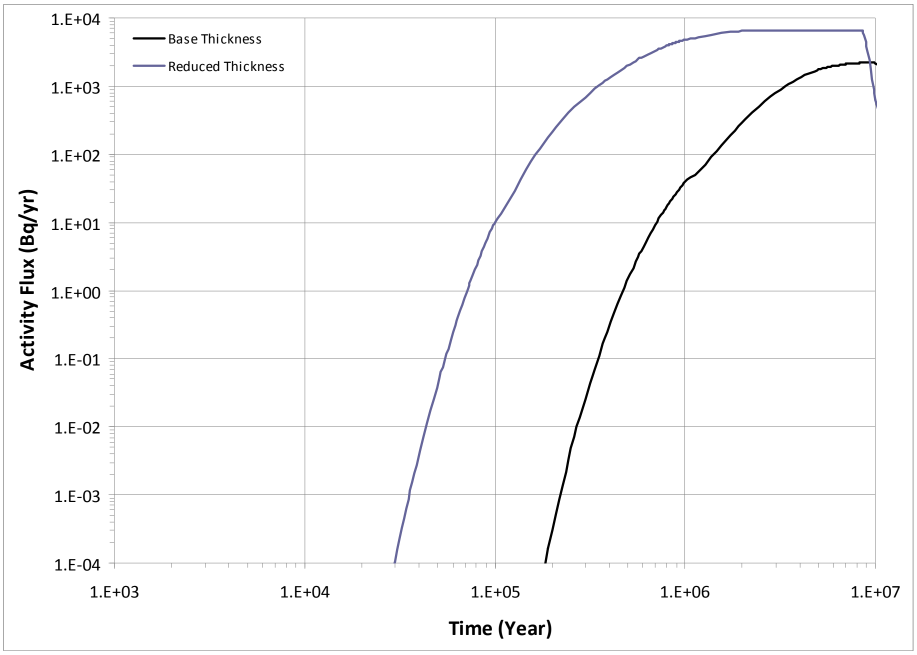
(b) PAMINA Benchmark



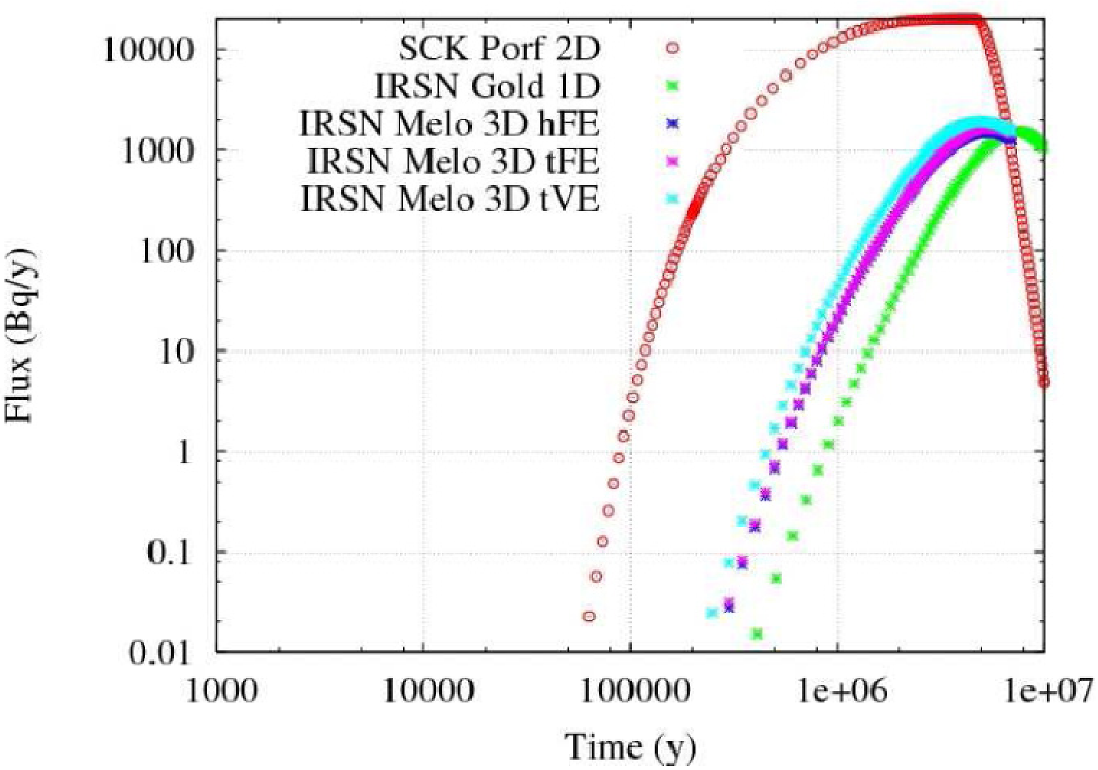
Source: Genty, Mathieu, and Weetjens 2009, Figure 17.

Figure 3.3-20. Np Activity Flux to Upper Aquifer– PAMINA Benchmark

(a) Clay GDS Model



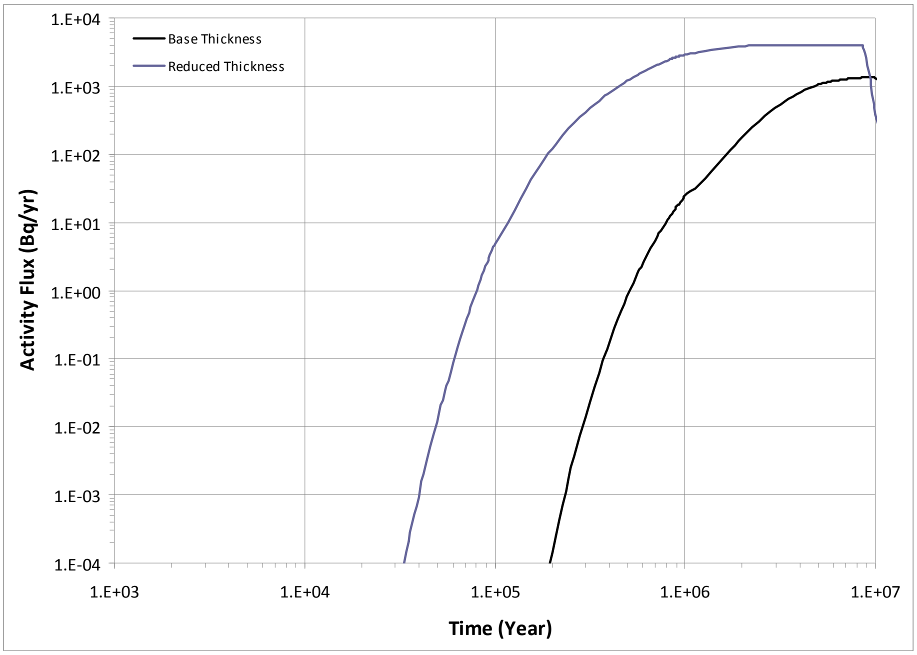
(b) PAMINA Benchmark



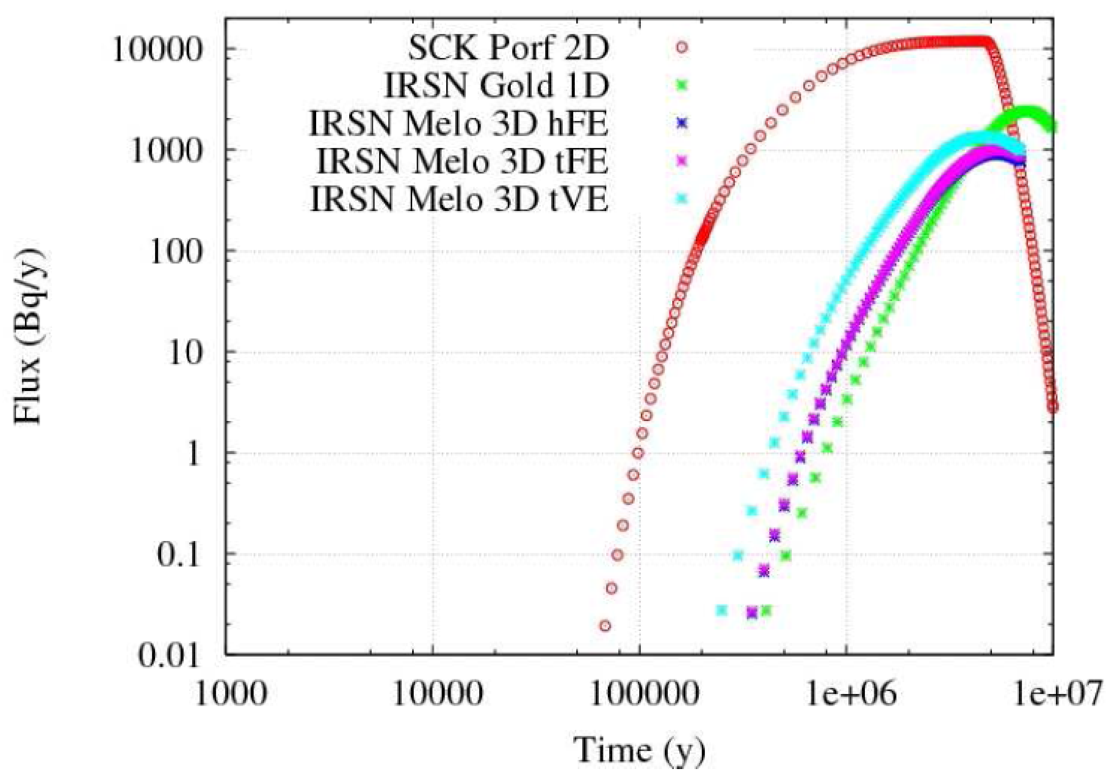
Source: Genty, Mathieu, and Weetjens 2009, Figure 18.

Figure 3.3-21. U Activity Flux to Upper Aquifer – PAMINA Benchmark

(a) Clay GDS Model



(b) PAMINA Benchmark



Source: Genty, Mathieu, and Weetjens 2009, Figure 17.

Figure 3.3-22. Th Activity Flux to Upper Aquifer – PAMINA Benchmark

3.3.3.3 Andra Dossier 2005 Argile

3.3.3.3.1 Purpose of Analysis

In 2005 Andra, France's National Radioactive Waste Management Agency, completed a series of feasibility assessment reports on clay formations (Dossier 2005 Argile) based on the work conducted on the site of the Meuse/Haute-Marne underground research laboratory. Part of this feasibility assessment included a safety assessment of a geologic repository. A variety of waste form types and inventories and a number of sensitivity analyses are documented. The current clay GDS model was used to reproduce the case of direct disposal of UNF (Case CU1).

3.3.3.3.2 Model Description

The following sources from the Andra Dossier 2005 Argile series were used to develop the clay GDS model representation:

- Architecture and Management of a Geologic Repository (Andra 2005a)
- Phenomenological Evolution of a Geologic Repository (Andra 2005b)
- Safety Evaluation of a Geologic Repository (Andra 2005c)

The configuration of the modeled disposal cells used is shown schematically in Figure 3.3-23 (Andra 2005a, Figure 5.2.17). The configuration parameters used are shown in Table 3.3-15.

The direct disposal of UNF analysis (Case CU1) considered the disposal of enriched uranium oxide fuels or enriched recycled uranium oxide fuels (Andra 2005c, Section 2.1.5). A total of 13,500 waste packages, each containing four used fuel assemblies were assumed in the calculation (Andra 2005c, Table 5.3-5). The radionuclide inventory used in the Andra Dossier 2005 safety evaluation considered 15 radionuclides, only fission or activation products. The reported inventory was for the entire 13,500 waste packages, and the reported inventory was not segregated between enriched uranium oxide fuels or enriched recycled uranium oxide fuels. In addition, only a limited number of actinides were only considered by Andra in sensitivity analyses to demonstrate that they do not contribute to repository performance over a 1,000,000-yr time period.

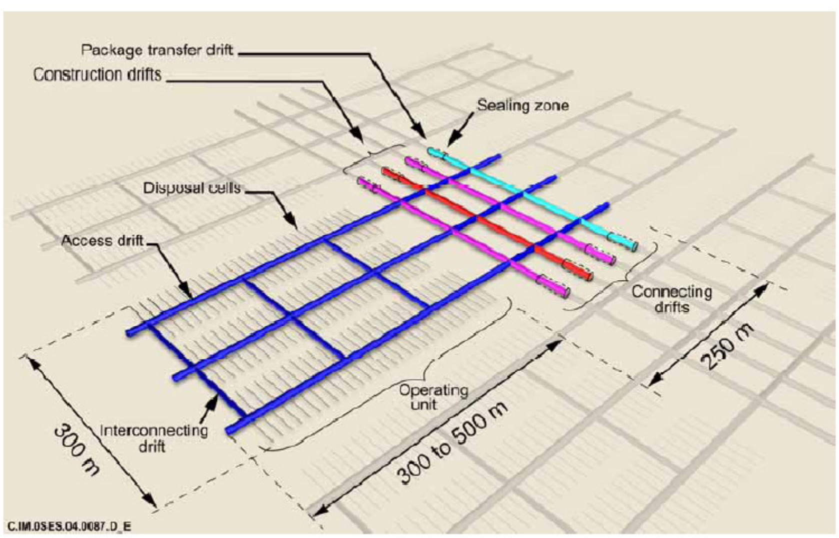


Figure 3.3-23. Andra Benchmark Configuration

Table 3.3-15. Andra Benchmark Configuration

Parameter	Value	Source
Domain Width (m)	5.5	[a]Section 5.2.4.1 (C panels: 8.5 - 13.5 waste package meter spacing, used average of 11 m)
Domain Height (m)	65	[b]Section 5.3.1.1, page 205
Domain Depth (m)	4.5	[b]Waste Package Length, Section 4.5

NOTE: [a]Andra 2005a
[b]Andra 2005c

In order to consider a full suite of radionuclides, the UNF radionuclide inventory was determined from the UFD *Fuel Cycle Potential Waste Inventory for Disposition* report (Carter, Luptak, and Gastelum 2011) for enriched uranium oxide PWR fuel assuming a burn-up of 60 GWd/MT, 30-yr cooled prior to disposal. Each waste package contains four UNF assemblies (~0.5 MT per assembly). The radionuclide inventory used is shown in Table 3.3-16. Also shown is a comparison of this inventory with the Andra Dossier 2005 Argile CU1 inventory for those radionuclides considered by Andra. This comparison shows that the inventory considered in the clay GDS model representation is very similar to that considered by Andra.

The EBS configuration modeled includes the waste form, the waste package, and a swelling clay secondary engineered barrier, consistent with that modeled in the Andra Dossier 2005 Argile safety evaluation (Andra 2005c). The Andra Dossier 2005 Argile safety evaluation assumed that the waste package (primary engineered barrier) failed 10,000 yr following repository closure and a subsequent gradual release of radionuclides from the UNF matrix over 50,000 yr following failure of the waste package (Andra 2005c, Section 5.3.2.1). A fractional degradation rate of 2×10^{-5} yr^{-1} was therefore used in the clay GDS model.

The waste package considered in the Andra Dossier 2005 was assumed to be unalloyed or weakly alloyed steel (Andra 2005c, Section 3.7.4.3) with an outer diameter of 1.25 m, a length of 4.5 m, and a thickness of 0.11 m (Andra 2005a, Section 4.3).

The properties of the degraded waste form and primary engineered barrier used are provided in Table 3.3-17. The degraded waste form density and porosity are assumed to be that of schoepite (Carter, Luptak, and Gastelum 2011, Table 6.3.8-6), although it is recognized that schoepite may not be the resultant product of UNF degradation in reducing conditions. However, no information could be found regarding these properties in the Andra Dossier 2005 Argile reports. The volume of the waste form batch-reactor mixing cell is assumed to equal the inner volume of the Andra waste package and the volume of the primary engineered barrier batch-reactor mixing cell is assumed to equal the volume of the waste package cylinder wall. The diffusive area for the diffusion area for the waste form and primary engineered barrier is assumed to equal the inner and outer cylinder areas, respectively, of the Andra waste package.

It was assumed that all radionuclides were infinitely soluble and nonsorbing in both the waste form and primary engineered barrier batch-reactor mixing cells. The Andra model also assumed infinite solubility and nonsorbing conditions in the waste form and EBS.

The advective flow rate through the waste form and the primary engineered barrier was assumed to equal the product of the far-field advective velocity (Darcy velocity) and the cross-sectional area (length×outer diameter) of each. The far-field advective velocity is discussed below.

Table 3.3-16. Radionuclide Inventory – Andra Benchmark

Isotope	[a]UFD Inventory (g/MT)	UFD Assembly Inventory (g/assembly)	UFD Waste Package Inventory (g/WP)	UFD Total Inventory (g/Repository)	UFD Total Activity Bq / Repository	[b]Andra Total Activity Scenario CU1 Bq/Repository	Activity Ratio (Andra / UFD)
^{227}Ac	3.96E-07	1.98E-07	7.92E-07	1.07E-02	2.86E+10		
^{241}Am	1.25E+03	6.25E+02	2.50E+03	3.38E+07	4.29E+18		
^{243}Am	2.71E+02	1.36E+02	5.42E+02	7.32E+06	5.40E+16		
^{14}C	4.54E-01	2.27E-01	9.08E-01	1.23E+04	2.03E+15	1.10E+15	0.54
^{36}Cl	5.01E-01	2.51E-01	1.00E+00	1.35E+04	1.65E+13	3.00E+13	1.82
^{245}Cm	9.54E+00	4.77E+00	1.91E+01	2.58E+05	1.64E+15		
^{135}Cs	7.72E+02	3.86E+02	1.54E+03	2.08E+07	8.88E+14	6.90E+14	0.78
^{137}Cs	1.05E+03	5.25E+02	2.10E+03	2.84E+07	9.09E+19		
^{129}I	3.13E+02	1.57E+02	6.26E+02	8.45E+06	5.10E+13	4.90E+13	0.96
^{93}Nb	7.13E+02	3.57E+02	1.43E+03	1.93E+07	2.01E+20		
^{237}Np	1.24E+03	6.20E+02	2.48E+03	3.35E+07	8.73E+14		
^{231}Pa	1.02E-03	5.10E-04	2.04E-03	2.75E+01	4.85E+10		
^{210}Pb	5.28E-01	2.64E-01	1.06E+00	1.43E+04	3.97E+16		
^{107}Pd	4.13E+02	2.07E+02	8.26E+02	1.12E+07	2.12E+14	1.80E+14	0.85
^{238}Pu	4.92E+02	2.46E+02	9.84E+02	1.33E+07	8.42E+18		
^{239}Pu	7.42E+03	3.71E+03	1.48E+04	2.00E+08	4.60E+17		
^{240}Pu	4.09E+03	2.05E+03	8.18E+03	1.10E+08	9.31E+17		
^{241}Pu	3.77E+02	1.89E+02	7.54E+02	1.02E+07	3.88E+19		
^{242}Pu	8.17E+02	4.09E+02	1.63E+03	2.21E+07	3.21E+15		
^{226}Ra	3.18E-06	1.59E-06	6.36E-06	8.59E-02	3.14E+09		
^{228}Ra	2.07E-12	1.04E-12	4.14E-12	5.59E-08	4.84E+05		
^{126}Sb	2.37E-06	1.19E-06	4.74E-06	6.40E-02	1.86E+17		

Table 3.3-16. Radionuclide Inventory – Andra Benchmark (continued)

Isotope	[a]UFD Inventory (g/MT)	UFD Assembly Inventory (g/assembly)	UFD Waste Package Inventory (g/WP)	UFD Total Inventory (g/Repository)	UFD Total Activity Bq / Repository	[b]Andra Total Activity Scenario CU1 Bq/Repository	Activity Ratio (Andra / UFD)
^{79}Se	1.05E+01	5.25E+00	2.10E+01	2.84E+05	1.33E+14	4.90E+14	3.68
^{126}Sn	4.99E+01	2.50E+01	9.98E+01	1.35E+06	1.41E+15	1.30E+15	0.92
^{90}Sr	4.44E+02	2.22E+02	8.88E+02	1.20E+07	6.05E+19		
^{99}Tc	1.28E+03	6.40E+02	2.56E+03	3.46E+07	2.17E+16	2.00E+16	0.92
^{229}Th	6.37E-06	3.19E-06	1.27E-05	1.72E-01	1.26E+09		
^{230}Th	2.28E-02	1.14E-02	4.56E-02	6.16E+02	4.70E+11		
^{232}Th	6.11E-03	3.06E-03	1.22E-02	1.65E+02	6.67E+05		
^{232}U	4.56E-03	2.28E-03	9.12E-03	1.23E+02	1.02E+14		
^{233}U	1.40E-02	7.00E-03	2.80E-02	3.78E+02	1.35E+11		
^{234}U	3.06E+03	1.53E+03	6.12E+03	8.26E+07	1.91E+16		
^{235}U	5.38E+03	2.69E+03	1.08E+04	1.45E+08	1.16E+13		
^{236}U	6.24E+03	3.12E+03	1.25E+04	1.68E+08	4.04E+14		
^{238}U	9.10E+05	4.55E+05	1.82E+06	2.46E+10	3.06E+14		
^{93}Zr	1.47E+03	7.35E+02	2.94E+03	3.97E+07	3.69E+15	2.80E+15	0.76
		0.5 MT/Assembly	[b]Four assemblies per waste package, Section 3.7.4.4, Figure 3.7-11	13,500 waste packages		[b]Table 5.3-5 (CU1)	

NOTE: [a] Carter, Luptak, and Gastelum 2011
[b] Andra 2005c
Shaded column used as input for the clay GDS model.
WP = waste package

The properties of the secondary engineered barrier (swelling clay) are provided in Table 3.3-18. The Andra Dossier 2005 Argile analyses considered a tunnel diameter of 3.3 m (Andra 2005a, Section 4.3). This gives a thickness of the swelling clay layer equal to 1.025 m. The waste package length (4.5 m) was used to determine the volume of the secondary engineered barrier batch-reactor mixing cell shown in Table 3.3-18.

No information could be found on the density or porosity of the swelling clay buffer. As such, the value of those parameters was assumed. The effective diffusion coefficients assumed by Andra in the swelling clay buffer were 5×10^{-10} m^2/s for all elements considered in the clay GDS model, except for C, Cl, I, Nb, and Se which were 5×10^{-12} m^2/s (Andra 2005c, Table 5.3-15). For a free water diffusion coefficient of 2.3×10^{-9} m^2/s (relative diffusivity of 1) and a porosity of 0.3, the tortuosity was set at 0.72 to yield the 5×10^{-10} m^2/s effective diffusion coefficient. The available porosity was set to 0.01 for C, Cl, I, Nb, and Se to yield the effective diffusion coefficient of 5×10^{-12} m^2/s. These values were also used in the clay GDS model.

Table 3.3-17. Waste Form and Primary Engineered Barrier Properties – Andra Benchmark

Property	Waste Form	Primary Engineered Barrier
Material Density (kg/m^3)	4830	5240
Porosity	0.175	0.4
Volume (m^3)	3.7	1.773
Thickness (m)	0.52	0.11
Diffusion Area (m^2)	14.6	17.7
Advective Flow Rate (m^3/yr)	3.55E-06	3.55E-06

Table 3.3-18. Secondary Engineered Barrier Properties – Andra Benchmark

Property	Secondary Engineered Barrier
Volume (m^3)	33.0
Thickness (m)	1.03
Perimeter (m)	10.4
Advective Flow Rate (m^3/yr)	9.37E-06
Porosity	0.3
Density (kg/m^3)	2300
Tortuosity	0.72
Fracture Spacing (m)	N/A
Fracture Aperture (m)	N/A

The advective flow rate through the swelling clay buffer (secondary engineered barrier) was assumed to equal the product of the far-field advective velocity (Darcy velocity) and the cross-sectional area (length×outer diameter) of the buffer. The far-field advective velocity is discussed below.

The dissolved concentration limits and distribution coefficients used were obtained from the Andra model and are shown in Table 3.3-19.

Table 3.3-19. Dissolved Concentration Limit and Distribution Coefficient Parameters – Swelling Clay Buffer, Andra Benchmark

Element	Dissolved Concentration Limit (Mol/L)	Distribution Coefficient (m^3/Kg)
Actinium	Infinitely Soluble	Nonsorbing
Americium	1.00E-10 [a]	1.20E+01 [a]
Antimony	Infinitely Soluble	Nonsorbing
Carbon	2.30E-03 [b]	Nonsorbing [c]
Cesium	Infinitely Soluble [a]	3.80E-01
Chlorine	Infinitely Soluble [b]	Nonsorbing
Curium	Infinitely Soluble	Nonsorbing
Iodine	Infinitely Soluble [a]	Nonsorbing
Lead	Infinitely Soluble	Nonsorbing
Neptunium	4.00E-09 [a]	1.00E+00 [a]
Niobium	2.00E-07 [b]	2.74E+02 [c]
Paladium	4.00E-07 [b]	3.43E+00 [c]
Protactinium	Infinitely Soluble	Nonsorbing
Plutonium	1.99E-07 [a]	1.00E+00 [a]
Radium	Infinitely Soluble	Nonsorbing
Selenium	5.00E-10 [b]	1.00E-03 [a]
Strontium	Infinitely Soluble	Nonsorbing
Technetium	4.00E-09 [b]	1.14E+02
Thorium	1.00E-09 [a]	3.00E+00 [a]
Tin	1.00E-08 [b]	4.19E+01 [c]
Uranium	5.00E-08 [a]	1.00E+02 [a]
Zirconium	2.00E-08 [b]	3.80E+02

NOTE: [a]Andra 2005b, Section 10.3.2.1
[b]Andra 2005c, Table 5.3-15
[c]Andra 2005c, Table 5.3.1-5 provides retardation coefficient, Kd determined from retardation coefficient, density, and porosity
Shaded elements – no information available, assumed infinitely soluble, nonsorbing.

The evolution of the EDZ is described in the Dossier 2005 Argile, *Phenomenological Evolution of a Geologic Repository* report (Andra 2005b, Section 8.2.3). The EDZ consists of a fractured zone in the immediate vicinity of the engineered structure and a microfissured zone behind the fractured zone. In a repository 500-m deep, Andra states that the fractured zone will extend for 15 centimeters and the microfracture zone will extend for over 1 m. The clay GDS model representation assumes an EDZ thickness of 1.15 m.

The properties of the EDZ are provided in Table 3.3-20. The Andra Dossier 2005 Argile analyses considered a tunnel diameter of 3.3 m (Andra 2005a, Section 4.3). This gives an outer diameter of the EDZ equal to 4.45 m. The waste package length (4.5 m) was used to determine the volume of the EDZ batch-reactor mixing cell shown in Table 3.3-20.

No information could be found on the density, porosity, and tortuosity of the EDZ. The porosity of the EDZ was assumed to equal that of the far field (discussed below) and the density was assumed to be 2,000 kg/m^3 (based on PAMINA benchmark properties discussed above).

The effective diffusion coefficient assumed in the clay GDS model was for the micro-fissure zone since it represented the greatest portion of the EDZ thickness. The effective diffusion coefficients assumed by Andra for the micro-fissure zone in the EDZ were 2.5×10^{-10} m^2/s for all elements considered in the clay GDS model, except for C, Cl, I, Nb, and Se which were 5×10^{-12} m^2/s (Andra 2005c, Table 5.3-14). For a free water diffusion coefficient of 2.3×10^{-9} m^2/s (relative diffusivity of 1) and a porosity of 0.18, the tortuosity was set at 0.6 to yield the 2.5×10^{-10} m^2/s effective diffusion coefficient. The available porosity was set to 0.02 for C, Cl, I, Nb, and Se to yield the effective diffusion coefficient of 5×10^{-12} m^2/s. These values were also used in the clay GDS model.

The advective flow rate through the EDZ was assumed to equal the product of the far-field advective velocity (Darcy velocity) and the cross-sectional area (length×outer diameter) of the EDZ. The far-field advective velocity is discussed below.

The dissolved concentration limits and distribution coefficients used were obtained from the Andra model and are shown in Table 3.3-21.

The properties of the far field are shown in Table 3.3-22. The far-field porosity is 0.18 (Andra 2005b, Table 3.3-1). The density was assumed to be 2,000 kg/m^3 (based on PAMINA benchmark properties discussed above).

Table 3.3-20. EDZ Properties – Andra Benchmark

Property	Secondary Engineered Barrier
Volume (m^3)	72.3
Thickness (m)	1.15
Perimeter (m)	17.6
Advective Flow Rate (m^3/yr)	1.59E-05
Porosity	0.18
Density (kg/m^3)	2000
Tortuosity	0.56
Fracture Spacing (m)	N\A
Fracture Aperture (m)	N\A

Table 3.3-21. Dissolved Concentration Limit and Distribution Coefficient Parameters – EDZ, Andra Benchmark

Element	Dissolved Concentration Limit (Mol/L)	Distribution Coefficient (m^3/Kg)
Actinium	4.00E-07[a]	5.00E+01[a]
Americium	4.00E-07[a]	5.00E+01[a]
Antimony	Infinitely Soluble	Nonsorbing
Carbon	2.30E-03[b]	4.14E-04[b]
Cesium	Infinitely Soluble[b]	4.00E-01[c]
Chlorine	Infinitely Soluble[b]	Nonsorbing[b]
Curium	4.00E-07[a]	5.00E+01[a]
Iodine	Infinitely Soluble[b]	Nonsorbing[b]
Lead	4.00E-06[a]	1.60E-01[a]
Neptunium	4.00E-09[a]	9.00E-01[a]
Niobium	2.00E-07[b]	4.81E+00[b]
Paladium	4.00E-07[b]	8.05E-01[b]
Protactinium	1.00E-06[a]	1.00E+00[a]
Plutonium	2.00E-07[a]	9.00E-01[a]
Radium	1.00E-07[a]	1.00E+00[a]
Selenium	5.00E-10[b]	Nonsorbing[b]
Strontium	Infinitely Soluble	Nonsorbing
Technetium	4.00E-09[b]	1.15E+00[b]
Thorium	6.00E-07[a]	8.00E+00[a]
Tin	1.00E-08[b]	1.61E+01[b]
Uranium	7.00E-07[a]	8.00E+00[a]
Zirconium	2.00E-08[b]	1.15E+00[b]

NOTE: [a]Andra 2005c, Table 5.5-5

[b]Andra 2005c, Table 5.3-14 provides retardation coefficient, Kd determined from retardation coefficient, density, and porosity

[c]Andra 2005c, Table 5.3.1-14 provides Cs Kd as a function of dissolved Cs concentration – assumed Cs concentration of 0 g/m^3 to determine Cs Kd

Shaded elements – no information available, assumed infinitely soluble, nonsorbing

Table 3.3-22. Far-Field Properties – Andra Benchmark

Property	Value
Porosity	0.18
Density (kg/m^3)	2000
Tortuosity : X-dimension	0.6
Tortuosity : Y-dimension	0.6

The effective diffusion coefficients assumed by Andra for the far field were 2.5×10^{-10} m^2/s for all elements considered in the clay GDS model, except for C, Cl, I, Nb, and Se which were 5×10^{-12} m^2/s (Andra 2005c, Table 5.3-16). For a free water diffusion coefficient of 2.3×10^{-9} m^2/s (relative diffusivity of 1) and a porosity of 0.18, the tortuosity was set at 0.6 to yield the 2.5×10^{-10} m^2/s effective diffusion coefficient. The available porosity was set to 0.02 for C, Cl, I, Nb, and Se to yield the effective diffusion coefficient of 5×10^{-12} m^2/s. These values were also used in the clay GDS model.

The advective velocity through the far field was 6.31×10^{-7} m/yr, based on a vertical hydraulic gradient of 5.0×10^{-14} m/s and a vertical hydraulic gradient of 0.4 (Andra 2005c, Table 5.5-1), and was consistent between the clay GDS model and Andra model.

The dissolved concentration limits and distribution coefficients used were obtained from the Andra model and are shown in Table 3.3-23.

3.3.3.3.3 Analysis Results

The annual dose from the Andra Dossier 2005 results and the clay GDS model are shown in Figure 3.3-24 for the CU1 case for the direct disposal of UNF (13,500 packages). Overall, the trends are similar. The peak annual dose occurs later for the clay GDS model. The peak annual dose is similar for ^{36}Cl and ^{79}Se and differs by a factor of approximately three for both radionuclides, with the clay GDS model results being lower. The magnitude of the peak annual dose for ^{129}I is a factor of 13 higher for the clay GDS model.

It must be recognized that the Andra Dossier 2005 Argile results allowed for both upward and downward vertical diffusion, explicitly represented radionuclide transport in overlying/ underlying formations as shown in Figure 3.3-25 (Andra 2005c, Figure 5.3-14), and included a detailed total-pathway representation of the biosphere. The difference in modeling diffusive transport alone would result in the clay GDS model over-estimating the resultant mass flux reaching the overlying aquifer by a factor of approximately two. The differences in modeling approaches for any surrounding formations and the biosphere would also contribute to the observed differences.

As such, the comparison between the peak annual dose should not be treated as an “absolute” difference, but are only used to demonstrate that the clay GDS model is not producing results that are “significantly” different (i.e., well over one order of magnitude). Based on this, the general tendencies are similar, and the comparisons of the clay GDS model and Andra results are excellent. This further indicates that the simplified representation of radionuclide transport in the clay GDS model is sufficient for the purposes of a generic simulation modeling tool of geologic disposal systems in clay.

Table 3.3-23. Dissolved Concentration Limit and Distribution Coefficient Parameters – Far-Field, Andra Benchmark

Element	Dissolved Concentration Limit (Mol/L)	Distribution Coefficient (m^3/Kg)
Actinium	4.00E-07[a]	5.00E+01[a]
Americium	4.00E-07[a]	5.00E+01[a]
Antimony	Infinitely Soluble	Nonsorbing
Carbon	2.30E-03[b]	4.14E-04[b]
Cesium	Infinitely Soluble[b]	4.00E-01[c]
Chlorine	Infinitely Soluble[b]	Nonsorbing[b]
Curium	4.00E-07[a]	5.00E+01[a]
Iodine	Infinitely Soluble[b]	Nonsorbing[b]
Lead	4.00E-06[a]	1.60E-01[a]
Neptunium	4.00E-09[a]	9.00E-01[a]
Niobium	2.00E-07[b]	4.81E+00[b]
Paladium	4.00E-07[b]	8.05E-01[b]
Protactinium	1.00E-06[a]	1.00E+00[a]
Plutonium	2.00E-07[a]	9.00E-01[a]
Radium	1.00E-07[a]	1.00E+00[a]
Selenium	5.00E-10[b]	Nonsorbing[b]
Strontium	Infinitely Soluble	Nonsorbing
Technetium	4.00E-09[b]	1.15E+00[b]
Thorium	6.00E-07[a]	8.00E+00[a]
Tin	1.00E-08[b]	1.61E+01[b]
Uranium	7.00E-07[a]	8.00E+00[a]
Zirconium	2.00E-08[b]	1.15E+00[b]

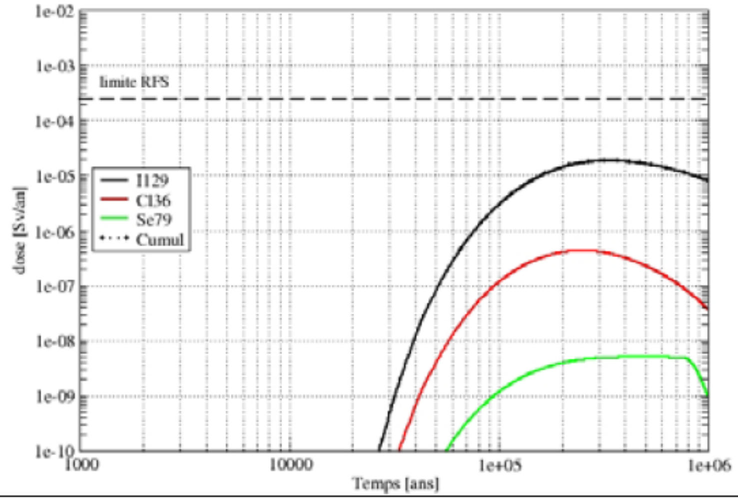
NOTE: [a]Andra 2005c, Table 5.5-5

[b]Andra 2005c, Table 5.3-16 provides retardation coefficient, Kd determined from retardation coefficient, density, and porosity

[c]Andra 2005c, Table 5.3.1-14 provides Cs Kd as a function of dissolved Cs concentration – assumed Cs concentration of 0 g/m3 to determine Cs Kd

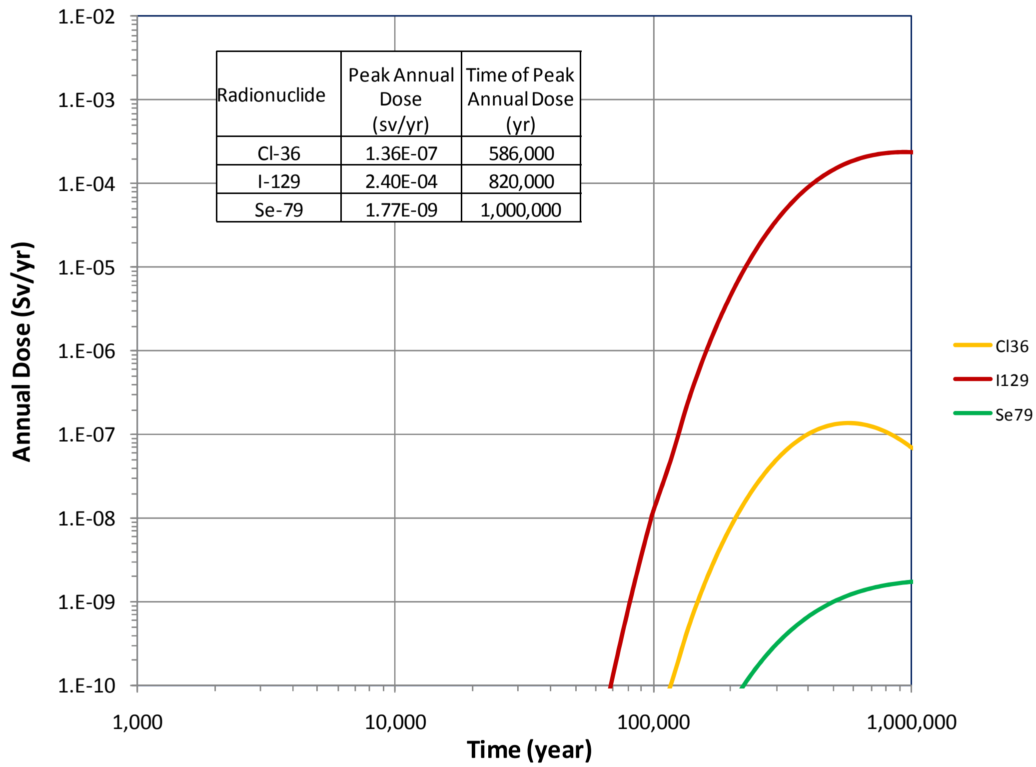
Shaded elements – no information available, assumed infinitely soluble, nonsorbing

(a) Andra Dossier 2005



RN	DoseMax[Sv/an]	t(DoseMax)[an]
Cumul	1.9E-05	3.3E+05
I129	1.8E-05	3.4E+05
Cl36	4.3E-07	2.5E+05
Se79	5.0E-09	4.7E+05

(b) Clay GDS Model



Radionuclide	Peak Annual Dose (sv/yr)	Time of Peak Annual Dose (yr)
Cl-36	1.36E-07	586,000
I-129	2.40E-04	820,000
Se-79	1.77E-09	1,000,000

Figure 3.3-24. Comparison of Andra Dossier 2005 Argile and Clay GDS Model Results

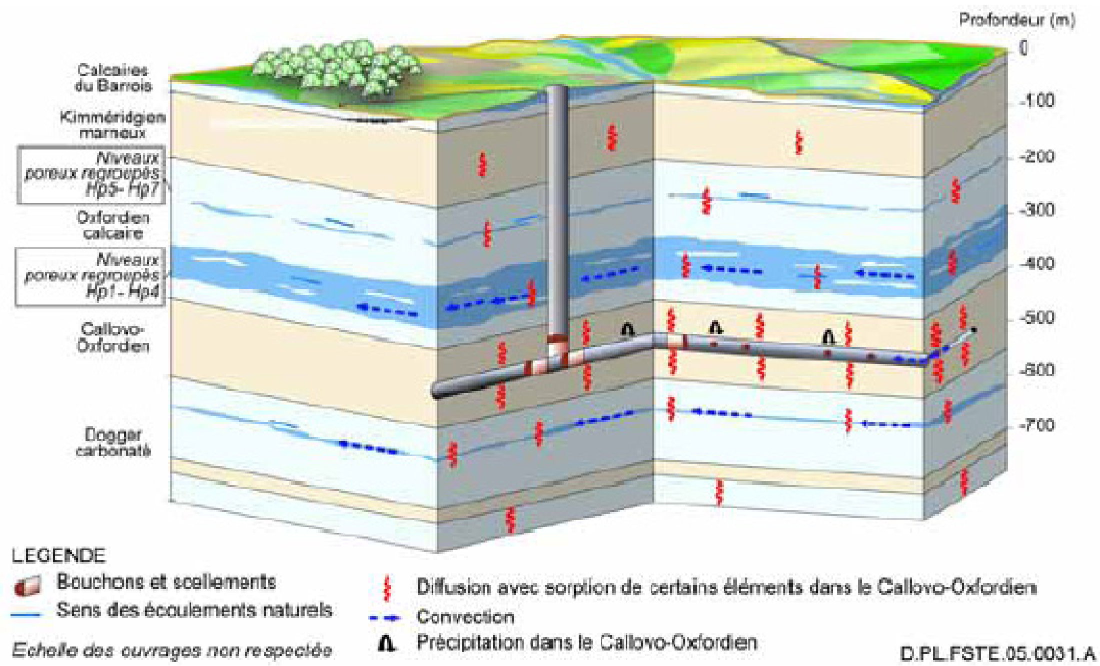


Figure 3.3-25. Schematic Diagram of Andra Dossier 2005 Argile Radionuclide Transport

3.3.4 Demonstration

This subsection describes the development of an "initial" concept and parameter set for a repository in a generic clay disposal environment. A limited set of sensitivity analyses are included to demonstrate the capability of the clay GDS model, beyond that shown in benchmark cases provided in Section 3.3.3.

3.3.4.1 Description of Initial Clay GDS Model Concept

The Andra Dossier 2005 Argile representation described in Section 3.3.3.3 served as a starting point for developing the initial clay GDS model concept. That representation was deterministic (single realization). The configuration and parameters provided in Section 3.3.3.3 were used, with the following changes:

- *Waste Form*—Assumed dissolved concentration limits were equal to that of the secondary engineered barrier. Assumed distribution coefficients from the *Total System Performance Assessment Model/Analysis for the License Application* for sorption onto degraded waste package internals (SNL 2008, Table 8.2-2).
- *Primary Engineered Barrier*—Assumed dissolved concentration limits were equal to that of the secondary engineered barrier. Assumed distribution coefficients from the *Total System Performance Assessment Model/Analysis for the License Application* for sorption onto degraded waste package internals (SNL 2008, Table 8.2-2).
- *Secondary Engineered Barrier (Swelling Clay Buffer)*—Set the minimum tortuosity and minimum available porosity a factor of 0.1 of the most likely value (Andra deterministic value). Set the maximum available porosity at 1. This allowed for a wide range of effective diffusive coefficients.
- *Secondary Engineered Barrier (Swelling Clay Buffer)*—Set the minimum and maximum dissolved concentration limits and distribution coefficients 2 orders of magnitude below/above the most likely value (Andra deterministic value).

- *EDZ*—Set the minimum tortuosity and minimum available porosity a factor of 0.1 of the most likely value (Andra deterministic value). Set the maximum available porosity at 1. This allowed for a wide range of effective diffusive coefficients.
- *EDZ*—Set the minimum and maximum dissolved concentration limits and distribution coefficients 2 orders of magnitude below/above the most likely value (Andra deterministic value).
- *Far Field*—Set the minimum tortuosity and minimum available porosity a factor of 0.1 of the most likely value (Andra deterministic value). Set the maximum available porosity at 1. This allowed for a wide range of effective diffusive coefficients.
- *Far Field*—Set the minimum and maximum dissolved concentration limits and distribution coefficients 2 orders of magnitude below/above the most likely value (Andra deterministic value).

Figure 3.3-26 shows the mean and median total annual dose along with the 5^{th}, 25^{th}, 75^{th}, 95^{th}, minimum and maximum for a 100-realization, 10,000,000-yr simulation of the clay GDS model using the “initial” parameter set discussed above. A 10,000,000-yr period was selected to capture the peak annual dose for all realizations given the properties selected for the “initial” parameter set. The results were normalized to MTHM of UNF disposed (2 MT per “waste unit cell”). The normalization was done because of the "waste unit cell" approach used in the clay GDS model. Simply reporting the annual dose as mrem/yr would be somewhat meaningless as it is the dose that would arise from a unit cell having 4 SNF assemblies, or 2 MT.

The radionuclides that contribute to the mean total annual dose are shown in Figure 3.3-27. The results are very similar those shown in Figure 3.3-24(b) with ^{129}I, ^{36}Cl, and ^{79}Se dominating the total dose in the “earlier” times (i.e., up to about 600,000 yr). When uncertainty is included, using the “initial” parameter set discussed above, in a stochastic simulation, ^{242}Pu, ^{135}Cs, and ^{237}Np also contribute over a 1,000,000-yr period. Other radionuclides also contribute over a longer time period.

Figure 3.3-28 shows the distribution of total annual dose for a 100-realization, 10,000,000-yr simulation of the clay GDS model using the “initial” parameter set discussed above at 100,000 yr; 1,000,000 yr; and 10,000,000 yr (i.e., slices out of Figure 3.3-27). A broad range, at very low annual doses, is seen at the 10,000-yr point. However, the variation decreases at later times, near where the peak annual dose occurs.

3.3.4.2 Sensitivity Analysis

A limited number of sensitivity analyses were conducted to further demonstrate the capabilities of the clay GDS model in evaluating the performance capabilities of a generic clay disposal environment. These sensitivity analyses use the median values of each of the “initial” parameter varies discussed above. Selected parameter values were varied as discussed below. Two groups of sensitivity analyses were conducted. The first considers the “nominal” disposal system and the second considers stylized hypothetical fast radionuclide transport pathway scenarios.

3.3.4.2.1 Nominal Sensitivity Analysis

The first sensitivity considers the effect of the time between reactor discharge of the UNF and when it is directly disposed of in the repository for PWR UNF with a burn-up of 60 GWd/MT. The results are shown in Figure 3.3-29. No sensitivity is seen. This is due to ^{129}I, with a half-life of 1.6×10^6 yr, being the dominant radionuclide and decaying very little up to 500 yr following reactor discharge.

The second sensitivity study evaluated the sensitivity to the waste form fractional degradation rate for PWR UNF with different burn-up, disposed of 30 yr following reactor discharge. The results, Figure 3.3-30, show a clear, essentially linear, dependence on burn-up. This is again because ^{129}I is the dominant radionuclide and as a fission product, its inventory in the used fuel is approximately a linear function of burn-up. The results also show that the performance of the waste form becomes more

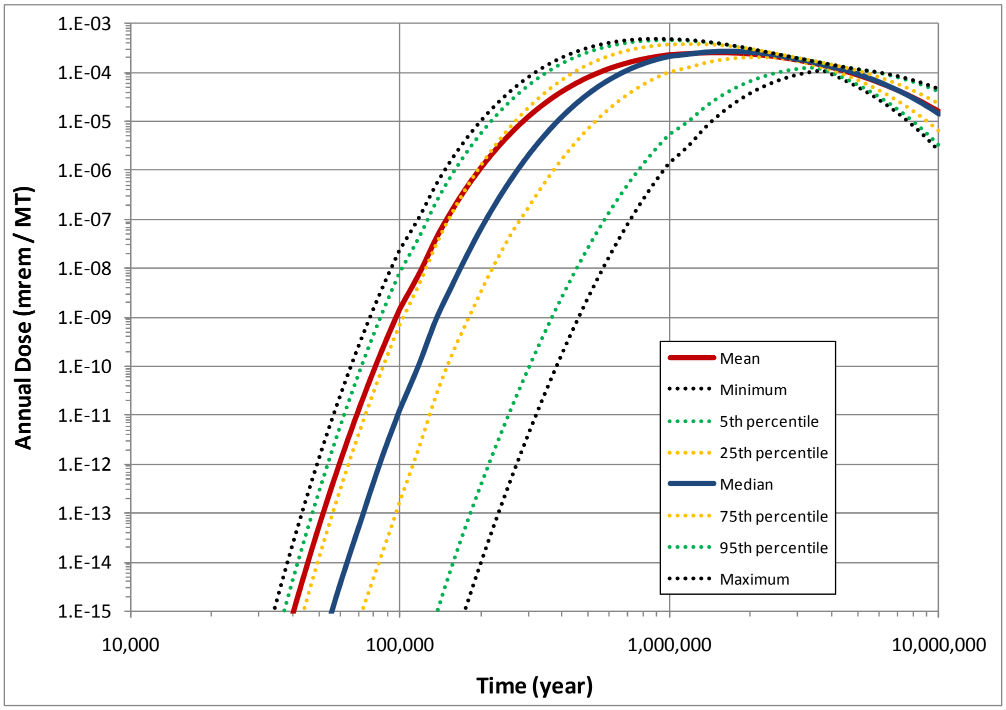


Figure 3.3-26. Time History of Total Annual Dose, Clay GDS Model – "Baseline" Parameter Set

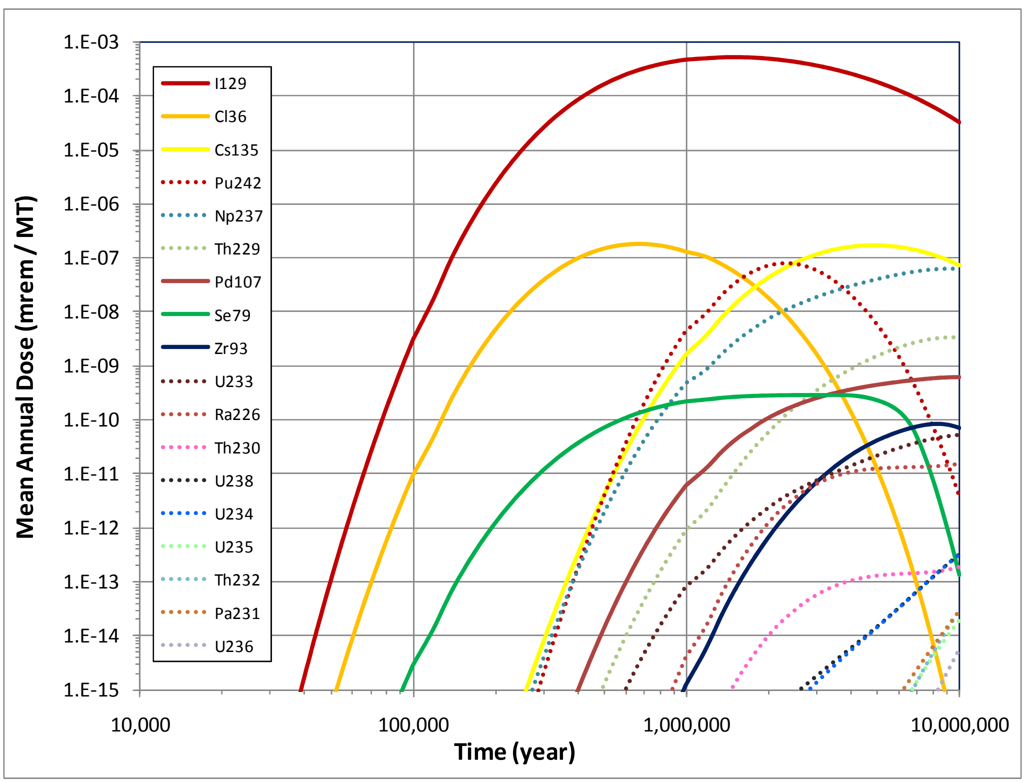


Figure 3.3-27. Radionuclide Contribution to the Mean Total Annual Dose, Clay GDS Model – "Baseline" Parameter Set

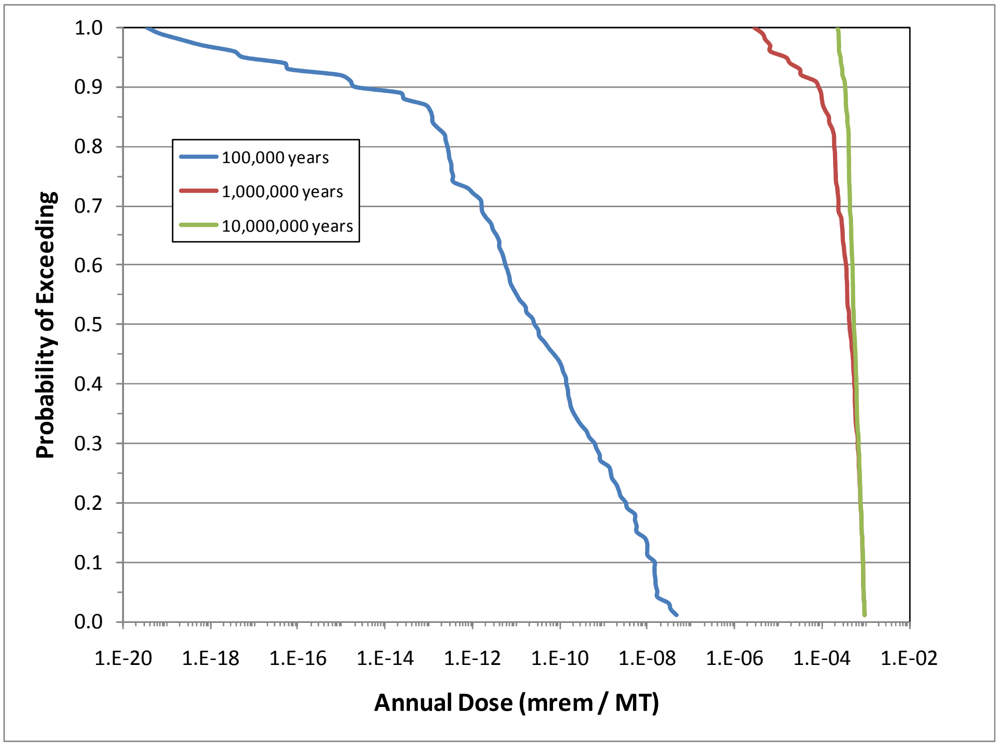


Figure 3.3-28. Distribution of Total Annual Dose, Clay GDS Model – “Baseline” Parameter Set

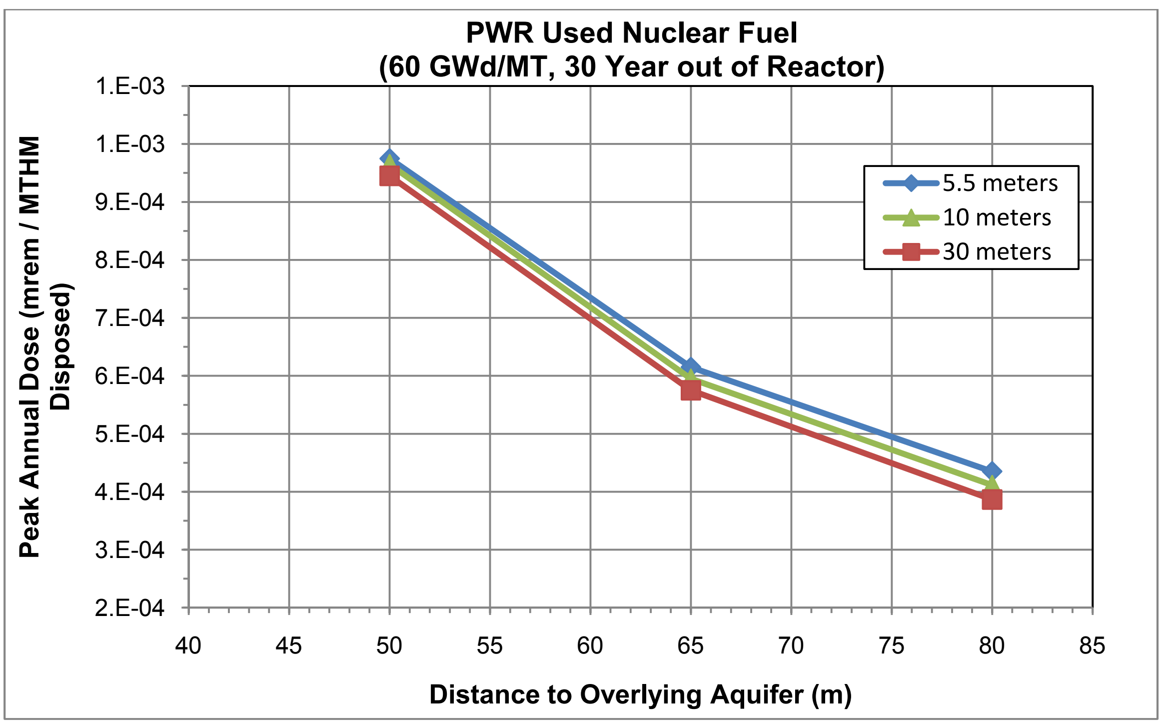


Figure 3.3-29. Clay GDS Model Sensitivity Analysis – Effect of UNF Decay

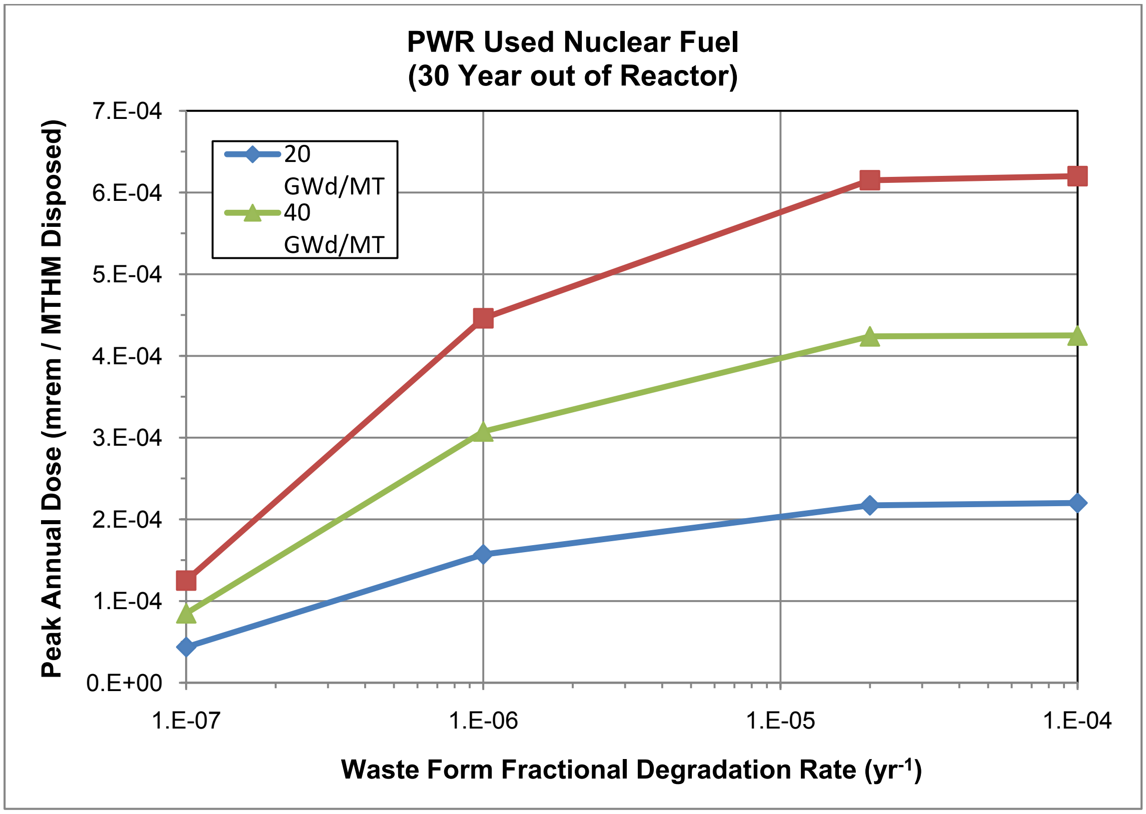


Figure 3.3-30. Clay GDS Model Sensitivity Analysis – Effect of UNF Burn-up and Fractional Degradation Rate

important as the fractional degradation rate decreases (waste form lifetime increases). At higher waste form degradation rates radionuclide release from the disposal system is controlled by radionuclide transport processes through the far field. As the waste form degradation rate decreases, the release of radionuclides from the EBS begins to contribute and the mass flux exiting the disposal system (and the annual dose) begins to decrease. At very low waste form degradation rates (approaching 1,000,000- to 10,000,000-yr waste form lifetimes), the releases from the waste form begin to dominate the release rate from the entire disposal system.

The third sensitivity analysis explores the effect of disposal system configuration by varying the distance between emplaced waste and the distance between the emplaced waste and an overlying aquifer. This was done by varying the width and height of the "waste unit cell" (Figure 3.3-3). The results are shown in Figure 3.3-31 and show very little sensitivity to the distance between emplaced waste, but strong sensitivity to the distance to an overlying aquifer. This shows that radionuclide transport is primarily 1D for the parameter set chosen.

The fourth sensitivity analysis evaluated the effects of increasing the vertical advective velocity (Darcy velocity) in the far field. The results, provided in Figure 3.3-32, show a transition where from where diffusive radionuclide transport controls the release of radionuclides to the overlying aquifer (and the annual dose) to where advective radionuclide transport begins to play a role, and, at higher velocities, begins to control the rate that radionuclides are released to the overlying aquifer.

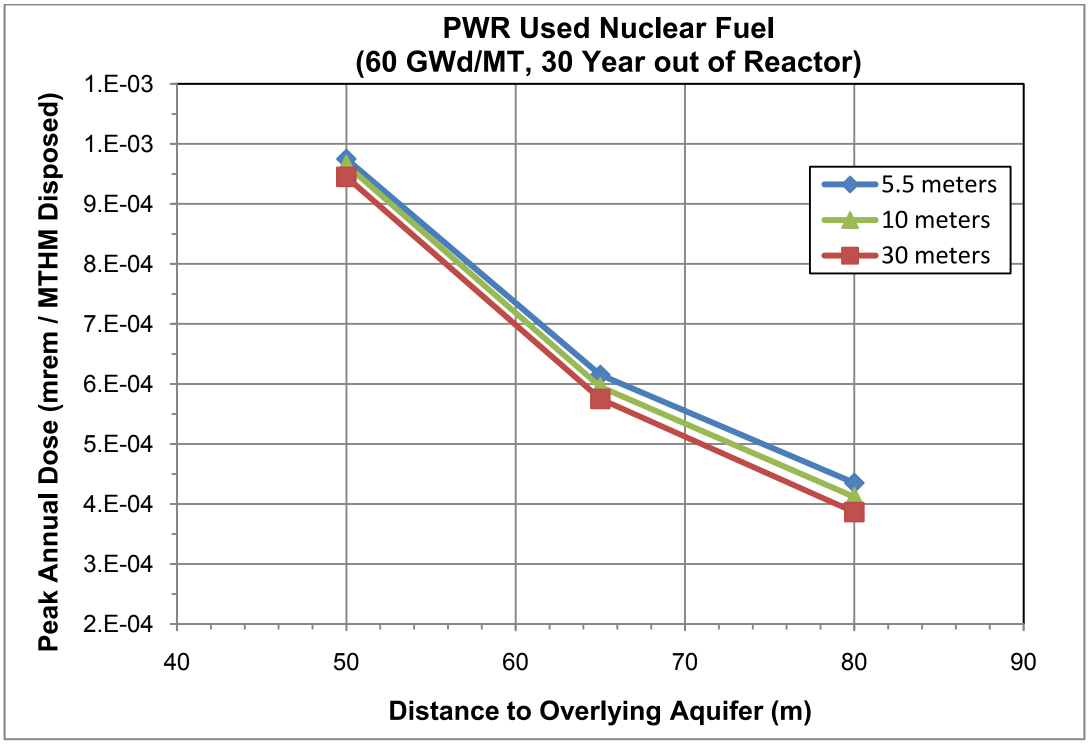


Figure 3.3-31. Clay GDS Model Sensitivity Analysis – Effect of Disposal System Configuration

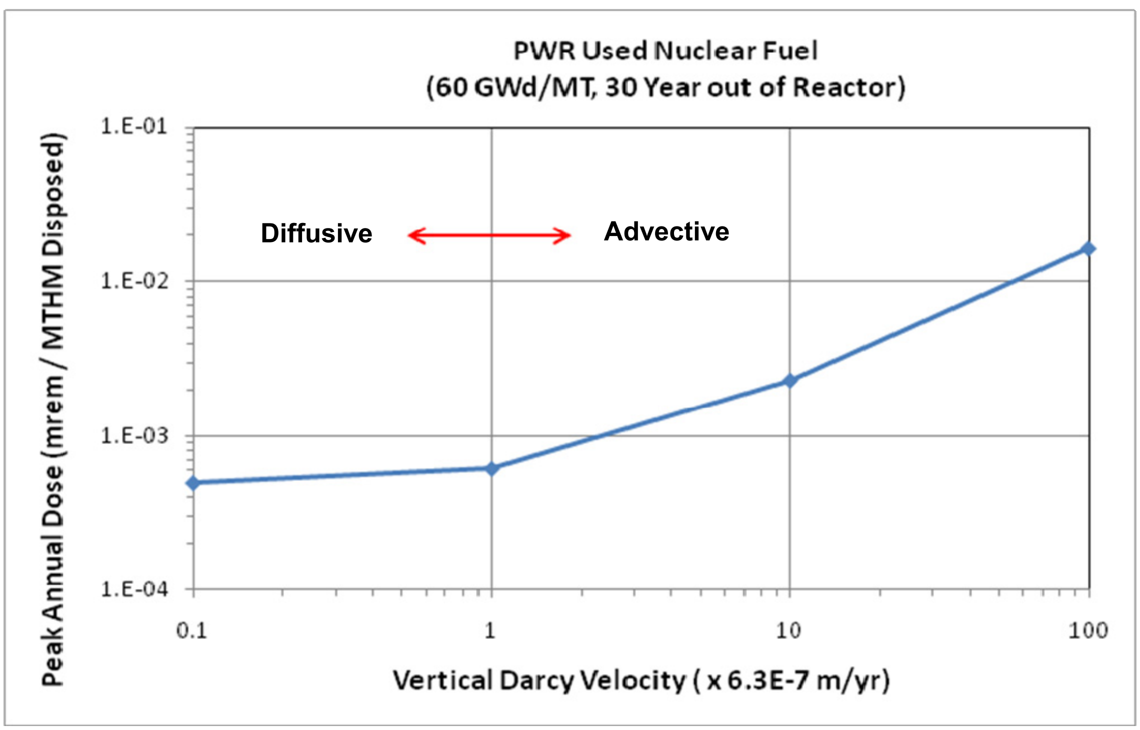


Figure 3.3-32. Clay GDS Model Sensitivity Analysis –
Effect of Far-Field Vertical Groundwater Velocity

3.3.4.2.2 Hypothetical, Fast Pathway Sensitivity Analysis

The first hypothetical fast pathway analysis considered an episodic advective pathway through the far field located 25% of the distance between the emplaced waste and the mid-plane between waste emplacement locations. The vertical ground water velocity (Darcy velocity) was assumed to flow episodically starting at 1,000,000 yr and continuing for 500,000 yr at varying rates. The results are shown in Figure 3.3-33. A significant sensitivity is seen only when the vertical groundwater velocity exceeds 100 times the "baseline" groundwater velocity (6.3×10^{-7} m/yr).

The second hypothetical fast pathway analysis considered an advective pathway directly intersecting the emplaced waste. No performance capability is ascribed to any engineered barriers and the radionuclide transport is assumed to occur via advective transport along a 65-m pathway to the overlying aquifer. The vertical groundwater velocity (Darcy velocity) was assumed to be 0.001 m/yr. The peak annual dose for this hypothetical scenario was very large, 1.33 rem/MT disposed, and as shown in Figure 3.3-34 dominated by ^{239}Pu and ^{240}Pu.

The third hypothetical fast pathway analysis built on that immediately above and included a 10-m diffusive pathway between the emplaced waste and the advective fast pathway. The cross-section for diffusion was assumed to equal 5 m^2. The properties of this diffusive zone were assumed to be identical to those of the EDZ discussed above. The free water diffusion coefficient was increased by an order of magnitude, leading to a 10-fold increase in the effective diffusion coefficient in this diffusive zone as compared to that of the EDZ discussed above. The peak annual dose for this hypothetical scenario was significantly lower than the direct advective intersection case discussed immediately above, 0.121 mrem/MT disposed. The radionuclides that contribute to the annual dose are shown in Figure 3.3-35, and are dominated by fission products. This shows that a relatively short diffusion zone between the emplaced waste and any advective fast pathway will result in a significant reduction in the release of radionuclides to an overlying aquifer.

The fourth hypothetical fast pathway analysis further builds on that immediately above and includes radionuclide transport through the degraded waste form, the primary engineered barrier, and secondary engineered barrier before entering the 10-m diffusive pathway between the emplaced waste and the advective fast pathway. The peak annual dose for this hypothetical scenario was again significantly lower than the case discussed immediately above, 0.05 mrem/MT disposed. The radionuclides that contribute to the annual dose are shown in Figure 3.3-36, and are dominated by fission products.

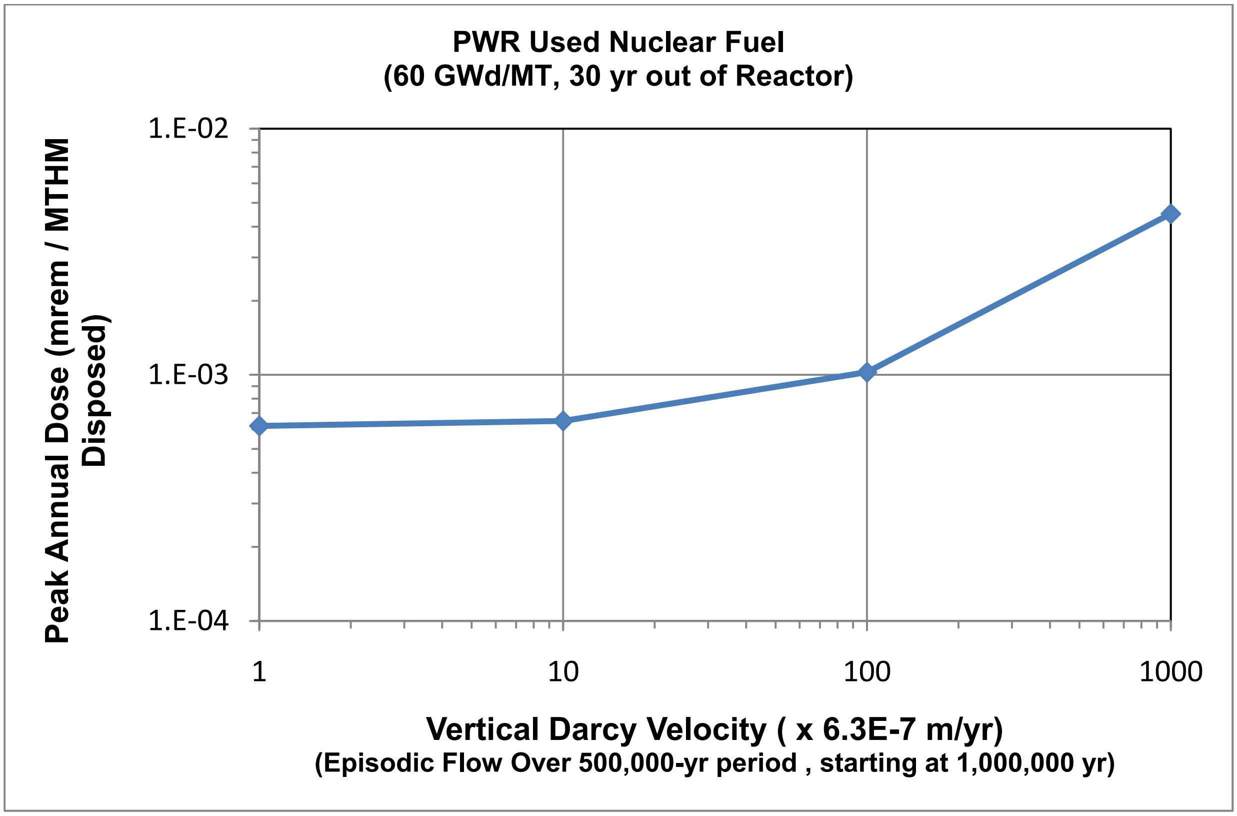


Figure 3.3-33. Clay GDS Model Sensitivity Analysis –
Episodic Far-Field Advective Transport Fast Pathway

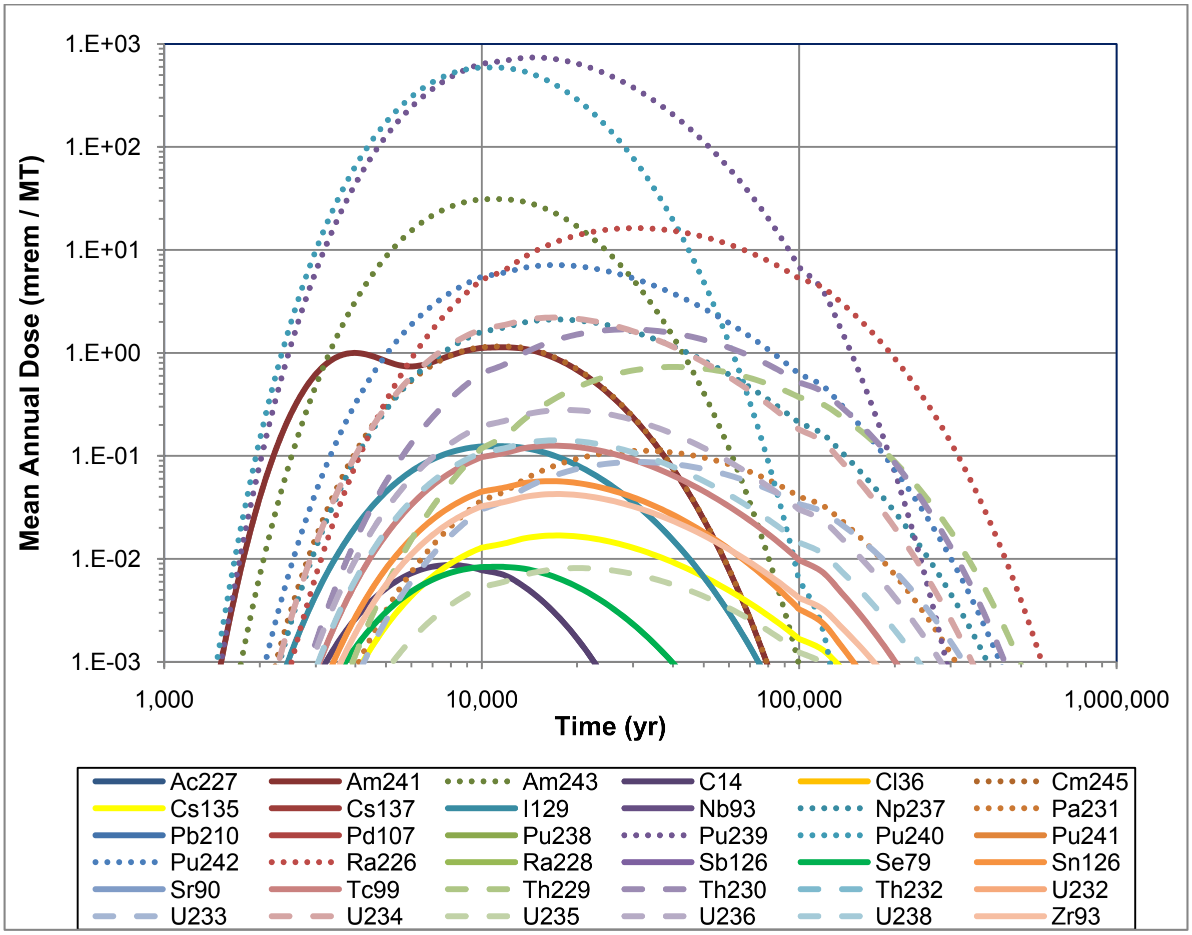


Figure 3.3-34. Clay GDS Model Sensitivity Analysis –
Hypothetical Direct Fast Pathway Intersection with Emplaced Waste

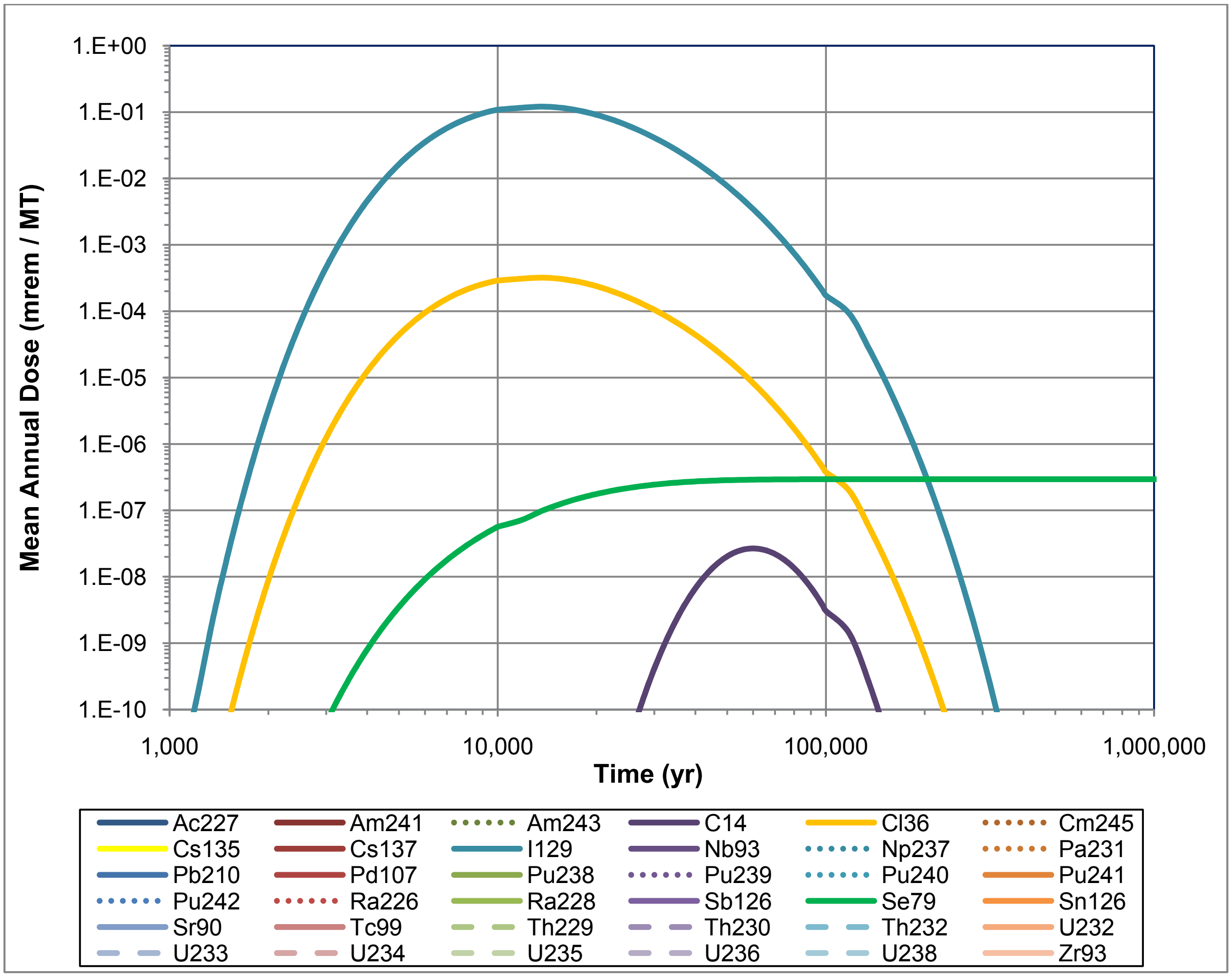


Figure 3.3-35. Clay GDS Model Sensitivity Analysis –
Hypothetical Diffusive and Advective Fast Pathway

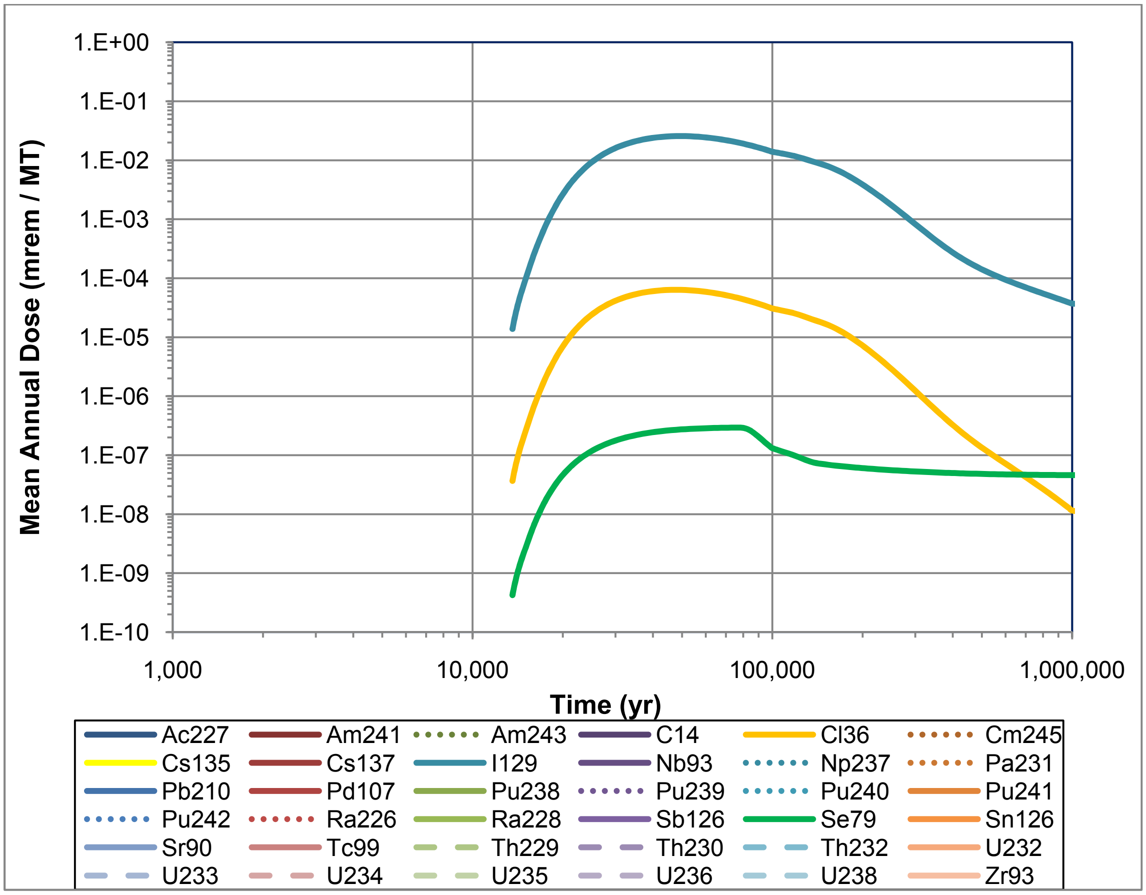


Figure 3.3-36. Clay GDS Model Sensitivity Analysis – Hypothetical Diffusive and Advective Fast Pathway Including Engineered Barriers

3.3.5 Conclusion

A clay GDS repository performance simulation tool has been developed with the flexibility to evaluate not only different properties, but different waste streams/forms and different repository designs and engineered barrier configurations/ materials that could be used to dispose of these wastes. Sections 3.3.1 through 3.3.4 describe that model, the clay GDS model, and demonstrate how the tool could be used both within the UFD Campaign and the broader FCT Program to do the following:

- Inform the prioritization of R&D activities within the UFD Campaign
- Provide metric information regarding waste management that could be used by the FCT systems engineering effort in evaluating various advanced fuel cycle alternatives
- Provide metric information to the FCT System Analysis Campaign in the development of fuel cycle system analysis tools.

This is the first version of a full-capability clay GDS model. It is expected that as research and development activities continue in both the UFD Campaign and the FCT Program, the capability to model a generic clay repository will be revised, as necessary, to incorporate additional detail to better represent key processes. These improvements will be made to the GPAM described in Section 4 rather than to the clay GDS model since the GPAM is incorporating the capability to model each of the salt, granite, clay, and deep borehole concepts. Such improvements could include:

- Representation of the coupled thermal-hydrologic-chemical processes to quantify the time-dependent evolution of the environment in the EBS and near field (EDZ).
- Improved representation of waste form degradation processes to better reflect any temporal variations in the fractional degradation rate and any other couplings between the degrading waste forms and the rest of the engineered barriers.
- Inclusion of multiple radionuclide release processes from degrading waste forms (i.e., surface and/or grain boundary release).
- Improved representation of primary engineered barrier degradation to include multiple degradation processes and couplings with the evolving EBS environment.
- Coupling of dissolved concentration limits and distribution coefficients to the evolving EBS and near-field (EDZ) environment.

3.4 Deep Borehole GDS Model

The development of the deep borehole GDS model is discussed in the subsections of Section 3.4. For consistency between generic disposal environments, many of the assumptions about model configurations developed for the salt GDS model (Section 3.1) and the granite GDS model (Section 3.2) were also applied to the deep borehole GDS model.

3.4.1 Model Description

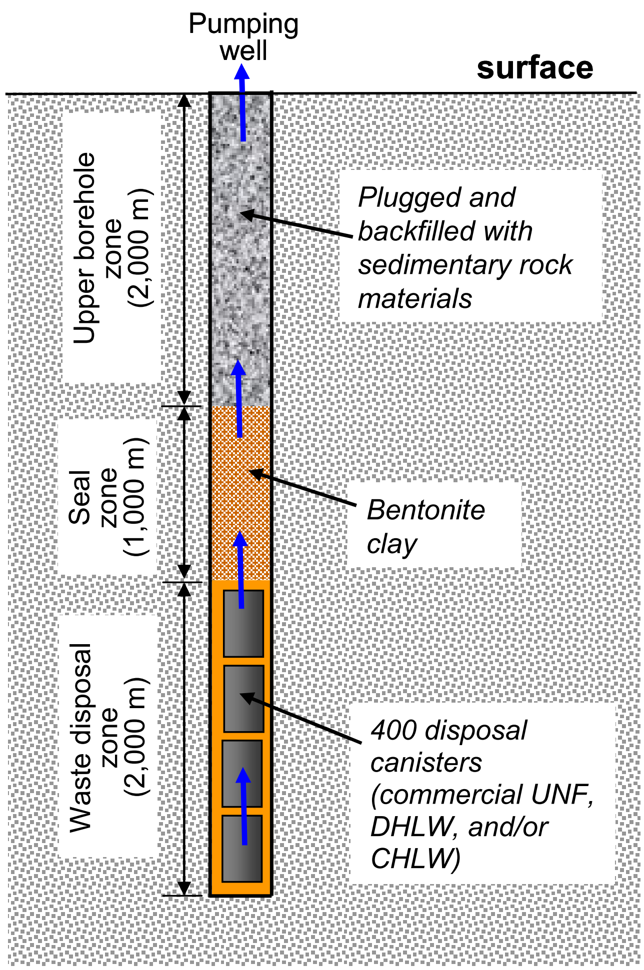
The deep borehole disposal concept consists of drilling deep boreholes into crystalline rocks for permanent disposal of high level radioactive waste. The conceptual model adopted for this study includes drilling boreholes to a depth of 5 km, emplacing waste packages in the lower 2 km, and constructing robust seals over 1-km length above the waste. The upper 2 km of the deep borehole are plugged and backfilled. The disposal concept relies on the presence of crystalline basement at many stable continental locations, and on existing drilling technology to construct boreholes at an acceptable cost. The additional advantages of this concept are that migration of radionuclides from the deep borehole would be severely restricted by the low permeability and high-salinity in deep crystalline rocks, limited interaction of deep fluids with shallower groundwater, and geochemically reducing conditions at depth, which limit the solubility and enhance the sorption of many radionuclides. An additional advantage that this option offers is the ability to dispose of nuclear materials incrementally and at distributed locations throughout the United States. Further description and analysis of the disposal concept can be found in Brady et al. (2009), Swift et al. (2011) and Arnold et al. (2011).

The deep borehole GDS model was implemented in GoldSim software (GoldSim Technology Group 2010b), and consists of three zones as shown in Figure 3.4-1:

- *Waste Disposal Zone*—Zone in the lower 2 km of the 5-km-deep borehole where the waste is emplaced. Waste packages are surrounded by bentonite grout and strings of canisters are separated by bridge plugs and compressed bentonite plugs.
- *Seal Zone*—Zone extending 1 km over the waste disposal zone, where robust sealing materials (such as bentonite, asphalt, and concrete) are placed.
- *Upper Borehole Zone*—Zone located in the top 2 km of the disposal borehole. In the deep borehole GDS model, this zone is assumed to be connected to a surrounding aquifer. Any radionuclides that reach the top of the seal zone can enter an intersecting aquifer and be pumped and transported to the surface from a water supply well completed in the aquifer. For dose simulations, exposure is assumed to occur on the surface at the top of the borehole, directly above the waste.

In the deep borehole GDS model vertical fluid flow is driven by thermal hydrology as a result of decaying heat from the radioactive waste. For the waste disposal and seal zones the model uses vertical flux results from a 3D model of thermal hydrologic flow (Arnold et al. 2011). As shown in Figure 3.4-2, the 3D model considers thermal hydrology in the borehole and the surrounding host rock. For the upper borehole zone and the surrounding aquifer, a constant groundwater flow rate representing a pumping well was used.

The model uses the contaminant transport module of GoldSim (GoldSim Technology Group 2010b) and the vertical groundwater fluxes to simulate radionuclide migration to the biosphere. Flow and transport in the disposal and seal zones occur in 1 m^2 cross-sectional area that consist of the borehole, seals, disturbed rock zone and grout. For this analysis radionuclides transported out of the seal zone are released into an aquifer where they are mixed and diluted. The radionuclides are then transported to the surface by a groundwater withdrawal well, and radiological dose is calculated from the resulting radionuclide concentrations using dose conversion factors. Using assumed average surface temperature and geothermal gradient described in Section 3.4.1.3.1, the average ambient temperature for the disposal and seal zones would be around 100° C. Thus, solubility calculations for the disposal and seal zones were based on an isothermal condition of 100°C (Wang and Lee 2010, Table 5). Solubility calculations for the upper zone were based on 25°C temperature. Similar to the conceptualization for the salt and granite GDS models, radionuclide solubility calculations were based on the assumptions of reducing conditions in the disposal and seal zones, and less reducing conditions in the upper zone. Radionuclide sorption is modeled in all three zones. The deep borehole GDS model simulates different waste types and estimates radionuclide releases and mean annual radiation doses. Radionuclide inventories, heat output, and waste-form degradation rates representative of different waste types have been used and are consistent with the other models in this report. The current deep borehole GDS model does not include human intrusion scenarios as this was considered an unlikely possibility given the vertical orientation of the borehole and that the borehole is sealed over 3 km in depth. Human intrusion scenarios will be studied further in the future.



NOTE: Assumptions of lithology and stratigraphy of the host rock and near-surface bedrock can be found in Brady et al. (2009) and Arnold et al. (2011)

Figure 3.4-1. Schematic Illustration of Deep Borehole Disposal of Commercial UNF, DHLW, and/or CHLW Used in Deep Borehole GDS Model

3.4.1.1 Waste Form

Three different types radioactive waste are considered in the source-term model: commercial UNF, existing DHLW, and hypothetical CHLW, a result of reprocessing of commercial UNF. The deep borehole GDS model shares waste inventory and waste degradation data with the salt and granite GDS models (Sections 3.1.2.2 and 3.2.2.2.1), based on a once-through fuel cycle waste inventory analysis (Carter and Luptak 2010). However, the deep borehole GDS source term differs due to a different waste loading (assemblies per waste package) governed by the deep borehole disposal design.

3.4.1.1.1 Waste Form Inventory

Source-term and radionuclide inventory data used in the deep borehole GDS model are based on the detailed fuel cycle waste inventory analysis provided by Carter and Luptak (2010).

Commercial UNF Inventory— A total of 140,000 MTU UNF is estimated to be discharged from reactors (Carter and Luptak 2010). For the deep borehole GDS near-field model, this total commercial UNF inventory is represented by an equivalent inventory of 321,540 PWR assemblies. For the deep borehole source-term model a single waste package is assumed to only 1 PWR assembly. The radionuclide inventory for commercial UNF in the deep borehole GDS model is shown in Table 3.4-1. This commercial UNF inventory is similar to the inventory for the salt GDS model shown in Table 3.1-1, except that salt GDS inventory per waste package is based on 10 assemblies per waste package.

DHLW Inventory—All existing DHLW is assumed to be immobilized in borosilicate glass logs. For the deep borehole GDS model, the source-term inventory analysis uses the best-estimate projected total number of DHLW canisters documented in the fuel cycle inventory analysis report (Carter and Luptak 2010, Table 2-2); the best estimate projection is 25,016 canisters. Each deep borehole waste package is assumed to contain only one DHLW canister. The deep borehole radionuclide inventory for DHLW is the same as the per canister inventory for the salt GDS model shown in Table 3.1-2.

CHLW Inventory—The report by Carter and Luptak discusses several candidate reprocessing methods for commercial UNF and their potential waste streams (Carter and Luptak 2010, Section 4). CHLW is assumed to be immobilized in the same borosilicate glass logs as DHLW, but with greater concentrations of fission products than the DHLW. The total radionuclide mass of the CHLW is estimated to be 1,426 MT (after removing 99% of uranium and plutonium). With a radionuclide mass loading of 0.07 MT per canister, this is equivalent to a total of 20,276 canisters. The deep borehole GDS source-term model assumes that each waste package contains only one reprocessed waste canister. The deep borehole radionuclide inventory for CHLW is the same as the per canister inventory for the salt GDS model shown in Table 3.1-3.

3.4.1.1.2 Waste Form Degradation

Waste form degradation for the deep borehole GDS model is treated the same as for the salt GDS model (Section 3.1.2.5) and the granite GDS model (Section 3.2.2.2.2). For commercial UNF, the waste form is the UNF matrix, which is predominantly UO_2. For the DHLW and CHLW, the waste form is borosilicate glass. For both waste form types, the waste form degradation in the deep borehole GDS near field is modeled with an annual fractional degradation rate (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates for deep borehole GDS conditions. The deep borehole GDS is expected to be located in a chemically reducing zone with varying degrees of redox conditions of groundwater in contact with the waste form. The chemically reducing conditions for the deep borehole GDS are assumed to be the same conditions as for the salt GDS and the granite GDS. Therefore the same probabilistic degradation rate models for the UNF matrix and for the borosilicate glass were used (Section 3.1.2.5).

Table 3.4-1. Isotopic Inventory for Commercial UNF for Deep Borehole GDS Model

Isotope	Half Life (yr)	Fractional Mass Inventory	Isotope Mass per Assembly (g)
^{227}Ac	2.18E+01	2.7469E-13	1.1960E-07
^{241}Am	4.32E+02	8.7003E-04	3.7882E+02
^{243}Am	7.37E+03	1.8796E-04	8.1841E+01
^{14}C	5.71E+03	3.1524E-07	1.3726E-01
^{36}Cl	3.01E+05	3.4808E-07	1.5156E-01
^{245}Cm	8.50E+03	6.6221E-06	2.8833E+00
^{135}Cs	2.30E+06	5.3570E-04	2.3325E+02
^{137}Cs	3.01E+01	7.2561E-04	3.1593E+02
^{129}I	1.70E+07	2.1754E-04	9.4720E+01
^{93}Nb	1.36E+01	4.9591E-04	2.1592E+02
^{237}Np	2.14E+06	8.5892E-04	3.7398E+02
^{231}Pa	3.25E+04	7.1103E-10	3.0959E-04
^{210}Pb	2.26E+01	7.8324E-15	3.4103E-09
^{107}Pd	6.50E+06	2.8663E-04	1.2480E+02
^{238}Pu	8.77E+01	3.4170E-04	1.4878E+02
^{239}Pu	2.41E+04	5.1487E-03	2.2418E+03
^{240}Pu	6.54E+03	2.8427E-03	1.2377E+03
^{241}Pu	1.44E+01	2.6198E-04	1.1407E+02
^{242}Pu	3.76E+05	5.6750E-04	2.4709E+02
^{226}Ra	1.60E+03	2.2081E-12	9.6141E-07
^{228}Ra	6.70E+00	1.4339E-18	6.2431E-13
^{126}Sb	3.61E-05	1.6470E-12	7.1713E-07
^{79}Se	6.50E+04	7.2769E-06	3.1684E+00
^{126}Sn	1.00E+05	3.4663E-05	1.5092E+01
^{90}Sr	2.91E+01	3.0809E-04	1.3414E+02
^{99}Tc	2.13E+05	8.8739E-04	3.8638E+02
^{229}Th	7.90E+03	4.4252E-12	1.9267E-06
^{230}Th	7.54E+03	1.5838E-08	6.8961E-03
^{232}Th	1.41E+10	4.2412E-09	1.8466E-03
^{232}U	6.89E+01	3.1642E-09	1.3777E-03

Table 3.4-1. Isotopic Inventory for Commercial UNF for Deep Borehole GDS Model (continued)

Isotope	Half Life (yr)	Fractional Mass Inventory	Isotope Mass per Assembly (g)
^{233}U	1.59E+05	9.7002E-09	4.2235E-03
^{234}U	2.45E+05	2.1220E-04	9.2392E+01
^{235}U	7.04E+08	3.7329E-03	1.6253E+03
^{236}U	2.34E+07	4.3349E-03	1.8874E+03
^{238}U	4.46E+09	6.3215E-01	2.7524E+05
^{93}Zr	1.53E+06	1.0193E-03	4.4382E+02

3.4.1.2 Waste Package

The deep borehole disposal concept allows for emplacement of waste packages (disposal canisters) vertically stacked down the 2-km length of the disposal zone. Assuming a 5-m length waste package, 400 waste packages (each assumed to contain either one commercial UNF assembly or one borosilicate glass canister) could be emplaced in a single borehole. Current simulations are based only on one type of waste in a single borehole. Thus, separate simulations are carried out for different waste types. One of the simplifying assumptions taken in the PA simulations is that waste package failure occurs immediately after emplacement. Thus, for PA simulation purposes degradation of the waste package is not modeled, which tends to over-estimate release.

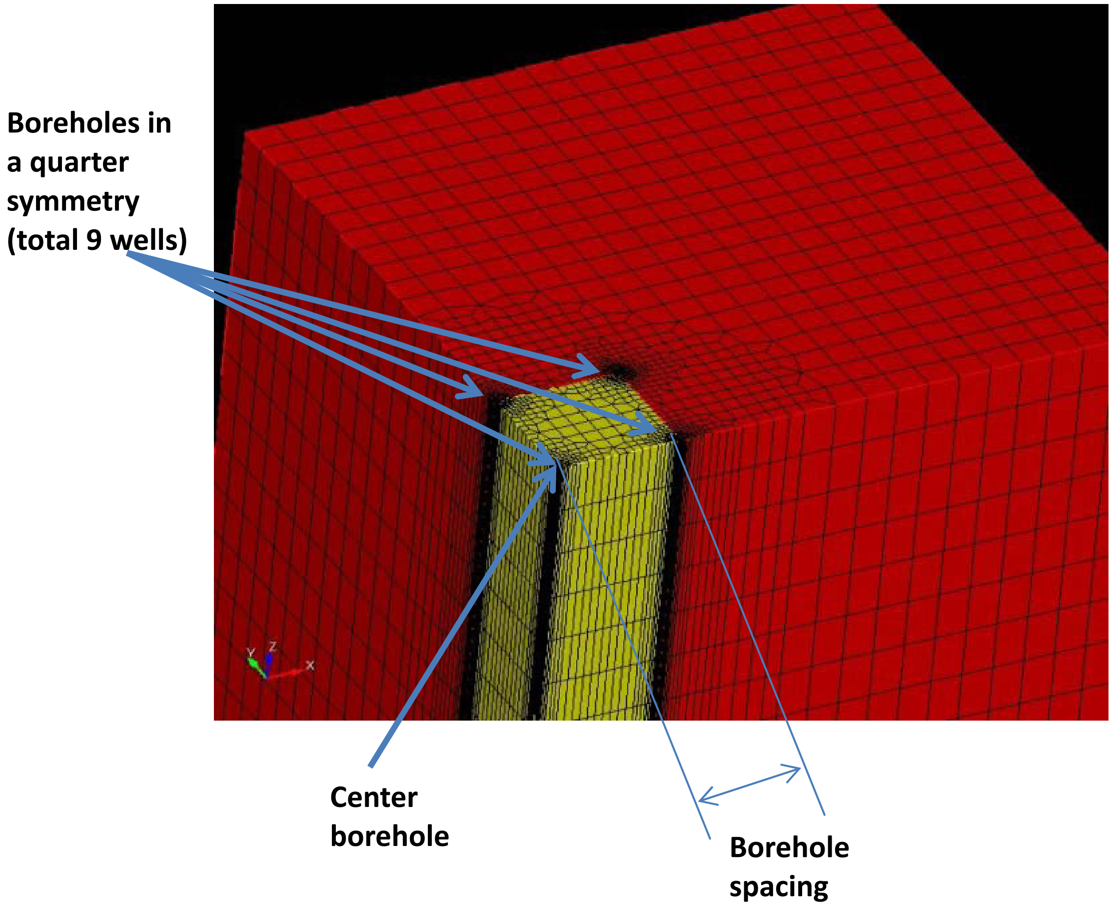
3.4.1.3 Inner EBS

For the deep borehole GDS model the inner EBS is represented by the waste disposal zone. This includes the waste package, the surrounding bentonite grout, and bridge plugs and compressed bentonite plugs that separate the strings of waste packages.

3.4.1.3.1 Evaluation of Vertical Fluid Flow: Thermal Hydrology Simulations

The deep borehole GDS model uses vertical fluxes obtained from an internal SNL deep borehole study (Arnold et al. 2011, Herrick et al. 2011). In the SNL study numerical simulations of thermal hydrology in the deep borehole disposal system were carried out with waste emplaced between 3000 m depth and the surface. The geometry of the system consisted of a disturbed zone of generally higher permeability than the host rock, within a cross-sectional area of 1 m^2 around the borehole, and low permeability host rock beyond the 1-m^2 cross-sectional area (Figure 3.4-2). For the simulations the seal material and the disturbed zone were represented with a single, combined, equivalent permeability and a total cross-sectional area of 1 m^2. The numerical grid uses a 3D model domain with quarter symmetry boundary conditions, and consists of hexahedral elements with higher resolution near the boreholes. For the simulations the base case set-up of 9 boreholes with borehole spacing of 200 m was used (Figure 3.4-2). For the simulation, the geothermal gradient was assumed to be 25°C/km and the average near-surface temperature was assumed to be 10°C.

Thermal-hydrologic simulations were conducted mainly for disposal of used commercial UNF assemblies but also for DHLW and CHLW canisters. Physical, thermal, and hydrologic properties representative of granite host rock at a depth of 4 km were used in the models shown in Table 3.4-2 (Brady et al. 2009, Table 3). Table 3.4-2 also shows bounding permeability values used in sensitivity analysis. The simulations were used to study temperature and fluid flow in the vicinity of the center borehole.



NOTE: Figure shows quarter symmetry for a system with 9 boreholes and 200-m borehole spacing.

Figure 3.4-2. Mesh Used for Thermal-Hydrologic Simulations

Table 3.4-2. Parameter Values Used in Thermal-Hydrologic Modeling

Parameter	Value
Thermal Conductivity (W/m ^{o}K)	3.0
Density (kg/m^3)	2750.
Porosity (-)	0.01
Specific Heat (J/kg ^{o}K)	790.
Base Case Permeability of Host Rock (m^2)	1×10^{-19}
Base Case Permeability of Seal/Disturbed Zone (m^2)	1×10^{-16}
Upper Bound Permeability of Host Rock (m^2)	1×10^{-16}
Upper Bound Permeability of Seal/Disturbed Zone (m^2)	1×10^{-12}
Lower Bound Permeability of Host Rock (m^2)	1×10^{-19}
Lower Bound Permeability of Seal/Disturbed Zone (m^2)	1×10^{-19}

The numerical model was implemented in the FEHM software code (Zyvoloski et al. 1997), and SNL's CUBIT software code was used for grid generation (SNL 2011). Figure 3.4-2 shows an illustration of the mesh generated using CUBIT. Thermal-hydrologic simulations were then carried out for a simulation time of 1,000,000 yr, with decay heat for three different waste types applied as a source of heat. The output of the simulations was thermally driven vertical fluxes for the waste disposal zone and the seal zone, at different depths and times. Figure 3.4-3 shows vertical ground water fluxes for commercial UNF waste at the depth of 3000 m, the top of the seal zone and 1,000 m above the top of the waste disposal zone. The curves represent results using the base case and bounding permeabilities. Note that for the base case and lower bound permeability cases, flows are downward between 1,000 and 10,000 yr.

3.4.1.3.2 Transport in the Disposal Zone

Radionuclide transport in the three deep borehole zones was modeled using the contaminant transport module of GoldSim (GoldSim Technology Group 2010b). Radionuclide transport processes modeled include advection, dispersion, diffusion, sorption, decay, and ingrowth. Advection resulted from thermally driven vertical water fluxes, as described in Section 3.4.1.3.1. Tabulated disposal zone vertical groundwater velocities obtained from the thermal-hydrologic simulations described in Section 3.4.1.3.1 were provided as input to the deep borehole GDS model. Ground water fluxes were tabulated in 100 m intervals from 3000- to 4000-m depth, and in 200-m intervals from 4000- to 5000-m depth, for times up to 1,000,000 yr. The ground water flux tables included disposal zone fluxes for the following cases:

- Commercial UNF waste with base permeability
- Commercial UNF waste with bounding high permeability
- DHLW with base permeability
- DHLW with bounding high permeability
- CHLW with base permeability

Note that radionuclide transport for the lower bound permeability case (Table 3.4-2) was not considered because of the very low vertical groundwater fluxes. Ground water velocities were then multiplied by the cross-sectional area of 1 m^2 to obtain volumetric flow rates. For transport simulations 20-m intervals were used over the disposal zone between depths of 3000 m and 5000 m. Note that even though the thermal-hydrologic calculations were based on nine wells to account for potential well thermal interactions, the deep borehole GDS model simulations are based on a single borehole. Probability distributions are used to describe the uncertainty in parameter values for the input parameters for waste form degradation rate, radionuclide solubility limits, and radionuclide sorption coefficients. Parameter values representative of the borehole disposal system and granite host rock are used for porosity, diffusion coefficient, effective dispersivity, bulk density, and waste package void volume. Linear sorption coefficients for reducing conditions were used for radionuclide retardation (Brady et al. 2009). Parameter values, including uncertainty distributions for parameters treated with uncertainty, are given in Table 3.4-3. Note that original sorption coefficient values were reduced by a factor of ten to account for the highly saline condition in the disposal zone. This is a conservative assumption as radionuclide sorption is reduced. Future simulations will be based on more representative sorption data.

Radionuclide solubility limits representative of geochemically reducing conditions in brine were applied (Brady et al. 2009) in the disposal zone. Solubility limits for the disposal zone were based on assumed isothermal conditions of 100°C (Section 3.4.1), representative of the average ambient temperature of deep granite, including uncertainty (Table 3.4-4).

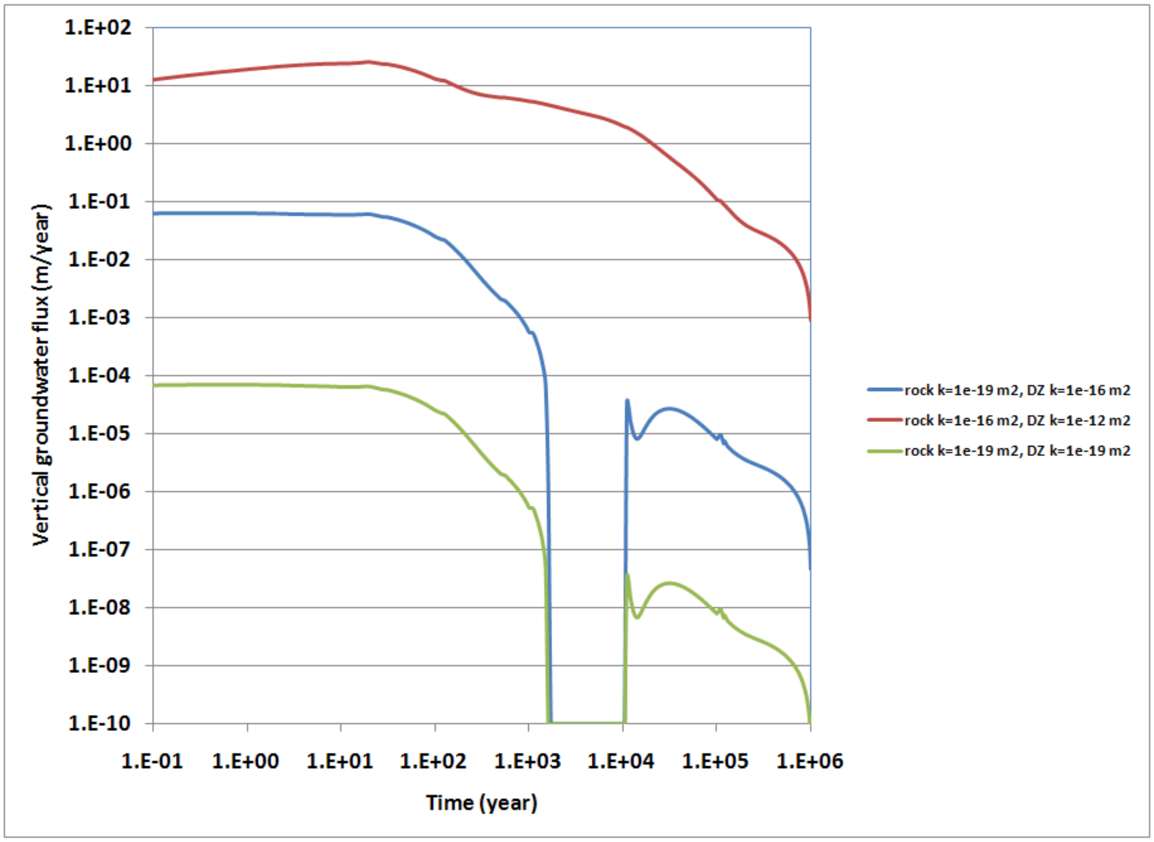


Figure 3.4-3. Vertical Groundwater Fluxes at Center of Corner Borehole Versus Time at 3000-m Depth for Base Case and Bounding Permeability Cases (Commercial UNF Waste)

Table 3.4-3. Transport Model Parameters for the Disposal Zone

Parameter	Distribution Type	Parameter Value and Description
Waste Disposal Zone		
Total length (m)	Constant	2,000
Cross sectional area (m^2)	Constant	1
Bulk density (kg/m^3)	Constant	2,450
Porosity	Constant	0.034
Tortuosity ($porosity^{1/3}$)	Constant	0.324
K_d for Radioelement (mL/g):		
Am, Ac, Cm	Log-uniform	5 (min); 5.0E+02 (max)
C	Uniform	0 (min); 0.6 (max)
Cs	Uniform	5 (min); 40 (max)
Np, Pa	Log-uniform	1 (min); 5.0E+02 (max)
Pu	Log-uniform	1 (min); 5.0E+02 (max)
Ra	Uniform	0.4 (min); 3 (max)
Sr	Uniform	0.4 (min); 3 (max)
Tc	Log-uniform	1.0E-05 (min); 25 (max)
Th	Log-uniform	3 (min); 5.0E+02 (max)
U	Log-uniform	0.4 (min); 5.0E+02 (max)
I	Uniform	0
Nb, Pd	Constant	1
Sb	Constant	10
Se	Uniform	0.2 (min); 0.5 (max)
Sn	Uniform	2 (min); 10 (max)
Zr	Log-uniform	3 (min); 5.0E+02 (max)
Cl, Pb	Constant	0

NOTE: Data in this table are from Brady et al. (2009). The Kd data for Nb, Pd, Sb, Se, Sn and Zr are from McKinley and Scholtis (1993). Original Kd values were reduced by a factor of 10 to account for sorption in a highly saline disposal zone.

Table 3.4-4. Radionuclide Element Solubility Values for the Disposal Zone in Concentrated Brine at 100°C (mg/L)

Element	Distribution Type	Solubility	Source
U	Triangular	9.916E-08 (min); 2.25E-07 (mode); 5.20E-07 (max)	Wang and Lee (2010)
Pu	Triangular	8.23E-09 (min); 8.23E-09 (mode); 9.03E-08 (max)	
Am	Triangular	1.90E-04 (min); 1.58E-03 (mode); 1.06E-02 (max)	
Np	Triangular	1.42E-01 (min); 4.49E-01 (mode); 1.42 (max)	
Th	Triangular	3.96E-03 (min); 7.82E-03 (mode); 1.58E-02 (max)	
Tc	Log-triangular	4.56E-05 (min); 1.33E-03 (mode); 3.91E-02 (max)	
Sn	Triangular	1.24E-03(min); 3.35E-03 (mode); 9.01E-03 (max)	
Ac	Constant	1.48E-03	Appendix C of this report
Cm	Constant	1.59E-03	
Cl	Constant	1.512E+05	
Nb	Constant	1.49	
Pa	Constant	4.39E-01	
Pd	Constant	4.28E+01	
Sb	Constant	7.94	
Se	Constant	1.58	
Zr	Constant	9.30E-06	
C, Cs, I, Ra, Sr	N/A	Unlimited solubility	

3.4.1.4 Outer EBS

In the deep borehole GDS model, the outer EBS is represented by the seal zone. Vertical groundwater velocities in the seal zone obtained from the thermal-hydrologic simulations (Section 3.4.1.3.1) were provided in tables as input to the deep borehole GDS model. Fluxes were tabulated in 100-m intervals from 2000- to 3000-m deep, for times out to 1,000,000 yr. The tables included seal zone fluxes for the following cases:

- Commercial UNF waste with base permeability
- Commercial UNF waste with bounding high permeability
- DHLW with base permeability
- DHLW with bounding high permeability
- CHLW with waste base permeability

As with the disposal zone, the seal zone velocities were multiplied by the cross-sectional area of 1 m^2 to obtain volumetric flow rates. For transport simulations 20 m intervals were used over the seal zone depths of 2000 m and 3000 m. Parameter values for the seal zone are given in Table 3.4-5. Transport simulations in the seal zone were carried out in a similar way as in the disposal zone. Linear sorption coefficients for reducing conditions were used for radionuclide retardation (Brady et al. 2009) without accounting for saline conditions because of the lower salinity at these elevations (Table 3.4-5). Solubility limits for the seal zone were based on assumed isothermal conditions of 100°C, as in the disposal zone. Thus, for the seal zone the same solubility data given in Table 3.4-4 were used.

Table 3.4-5. Transport Model Parameters for the Seal Zone

Parameter	Distribution Type	Parameter Value and Description
Seal Zone (Bentonite)		
Total length (m)	Constant	1,000
Cross sectional area (m^2)	Constant	1
Bulk density (kg/m^3)	Constant	2,450
Porosity	Constant	0.034
Tortuosity ($porosity^{1/3}$)	Constant	0.324
Kd for Radioelement (mL/g):		
Am, Ac, Cm	Log-uniform	300 (min); 2.94E+04 (max)
C	Constant	5
Cs	Log-uniform	120 (min); 1.0E+03 (max)
Np, Pa	Log-uniform	30 (min); 1.0E+03 (max)
Pu	Log-uniform	150 (min); 1.68E+04 (max)
Ra	Log-uniform	50 (min); 3.0E+03 (max)
Sr	Log-uniform	50 (min); 3.0E+03 (max)
Tc	Log-uniform	1 (min); 250 (max)
Th	Log-uniform	63 (min); 2.35E+04 (max)
U	Log-uniform	90 (min); 1.0E+03 (max)
Nb	Constant	10
Pd	Uniform	5 (min); 12 (max)
Sb	Constant	100
Se	Uniform	4 (min); 20 (max)
Sn	Uniform	17 (min); 50 (max)
Zr	Log-uniform	100 (min); 5.0E+03 (max)
Cl, I, Pb	Constant	0

NOTE: Data in this table are from Brady et al. (2009). The Kd data for Nb, Pd, Sb, Se, Sn and Zr are from McKinley and Scholtis (1993).

3.4.1.5 Aquifer

In the deep borehole GDS model the aquifer is assumed to be represented by the upper borehole zone. This can be conceptualized as an aquifer intersecting the deep borehole at a depth of 2,000 m with a withdrawal well located no distance from the deep borehole. This differs from the conceptualization of the withdrawal wells used in the salt, granite, and clay repositories where the withdrawal well is located 5 km away from the boundary of the repositories footprint. Transport in the upper borehole zone is carried out in a similar way as in the disposal and seal zones using the contaminant transport module of GoldSim (GoldSim Technology Group 2010b). However, a constant volumetric groundwater rate of 0.00235 m^3/yr was used for the upper zone. The rate was obtained as a result of an analysis varying groundwater rate to match the breakthrough curve (of pumping well for 1000 people) in Brady et al. (2009, Figure 11) using a

1D transport model. The analysis was done to ensure that the GoldSim 1D upper zone transport model represents the 2D groundwater pumping model used in Brady et al. (2009, Section 3.2.3). Note that use of such a constant pumping rate for the entire duration of the 1,000,000-yr simulation is one of the conservative assumptions of the simulation.

Parameter values for the upper borehole zone are given in Table 3.4-6. For the upper zone linear sorption coefficients for less reducing conditions (as compared to the disposal and seal zones) are used to account for radionuclide retardation in that environment. Solubility limits for the upper zone were based on assumed isothermal conditions of 25°C. The values in Table 3.4-6 are different from those used in the other GDS models documented in this report because parameter data for the upper borehole zone of the deep borehole GDS model originated from the SNL deep borehole study (Brady et al. 2009).

Table 3.4-6. Transport Model Parameters for the Upper Borehole Zone

Parameter	Distribution Type	Parameter Value and Description
Upper Zone (plugged and backfilled with sedimentary rock materials)		
Total length (m)	Constant	2,000.
Cross sectional area (m^2)	Constant	1
Bulk density (kg/m^3)	Constant	2,450
Porosity	Constant	0.01
Tortuosity ($porosity^{1/3}$)	Constant	0.215
Kd for Radioelement (mL/g):		
Am, Ac, Cm	Log-uniform	100 (min); 1.0E+05 (max)
C	Log-uniform	1 (min); 2.0E+03 (max)
Cs	Log-uniform	10 (min); 1.0E+04 (max)
Np, Pa	Log-uniform	10 (min); 1.0E+03 (max)
Pu	Log-uniform	300 (min); 1.0E+05 (max)
Ra	Log-uniform	5 (min); 3.0E+03 (max)
Sr	Log-uniform	5 (min); 3.0E+03 (max)
Tc	Log-uniform	0.1 (min); 1.0E+03 (max)
Th	Log-uniform	800 (min); 6.0E+04 (max)
U	Log-uniform	20 (min); 1.7E+03 (max)
Nb	Constant	10
Pd	Uniform	4 (min); 100 (max)
Sb	Constant	100
Se	Uniform	1 (min); 8 (max)
Sn	Log-uniform	50 (min); 700 (max)
Zr	Log-uniform	100 (min); 8.3E+03 (max)
Cl, I, Pb	Constant	0

NOTE: Data in this table are from Brady et al. (2009). The Kd data for Nb, Pd, Sb, Se, Sn and Zr are from McKinley and Scholtis (1993).

Table 3.4-7. Radionuclide Element Solubility Values for the Upper Borehole Zone at 25°C (mg/L)

Element	Distribution Type	Solubility (molal)	Source
U	Triangular	2.18E+01 (min); 6.29E+01 (mode); 1.81E+02 (max)	Wang and Lee (2010)
Pu	Triangular	1.89E-01 (min); 6.25E-01 (mode); 2.07 (max)	
Am	Triangular	8.11E-02 (min); 2.56E-01 (mode); 8.11E-01 (max)	
Np	Triangular	2.62E-01 (min); 2.62 (mode); 2.62E+01 (max)	
Th	Triangular	2.05 (min); 4.09 (mode); 8.16 (max)	
Sn	Triangular	2.25E-03 (min); 6.05E-03 (mode); 1.63E-02 (max)	
Ac	Constant	2.41E-01	Appendix C of this report
Cm	Constant	2.60E-01	
Cl	Constant	1.51E+05	
Nb	Constant	1.49	
Pa	Constant	2.56	
Pd	Constant	4.28E+01	
Sb	Constant	7.94	
Se	Constant	1.58	
Zr	Constant	9.30E-06	
C, Cs, I, Ra, Sr	N/A	Unlimited solubility	

3.4.1.6 Receptor

In the deep borehole GDS model radionuclides transported out of the seal zone are released into an aquifer (the upper zone) where they are mixed and diluted. The radionuclides are then transported to the surface by a groundwater withdrawal well. In this study exposure is assumed to occur on the surface at the top of the borehole, directly above the upper zone. The IAEA's BIOMASS ERB 1B dose model (IAEA 2003) is used to convert the dissolved radionuclide concentrations in groundwater to an estimate of annual dose to a receptor based on drinking well water consumption. The model uses a dilution rate of 10,000 m^3/yr to account for the fact that the borehole water would mix with water in an existing aquifer before it was captured by the withdrawal well (assumed to supply 1,000 people). An individual water consumption rate of 1.2 m^3/yr has been used (IAEA 2003). Further discussion of the IAEA model can be found in Section 3.1.2.8.

3.4.2 Confidence Building and Demonstration of Capability

3.4.2.1 Confidence-Building Exercise: 1D Transport in the Seal Zone

As part of a confidence-building exercise, the deep borehole GDS model was compared with an analytical solution for advection-dispersion transport. For the exercise the PA analysis described in Brady et al. (2009, Section 5) has been adopted with some simplifications. In the exercise radionuclide transport up the seal zone from the waste disposal zone occurs for a period of 200 yr, corresponding to the duration of the thermally driven flow (Brady et al. 2009, Figure 8). Thus, the total time for the simulation is 200 yr. Since iodine was found to be the dominant contributor to dose (Brady et al. 2009, Section 5), this exercise focuses on iodine transport only. The analytical solution implemented in Brady et al. (2009, Section 5) is based on the Ogata-Banks solution for 1D advection-dispersion from a continuous source with retardation and radioactive decay (Domenico and Schwartz 1990, Equation 17.10).

Equation 3.4-2 gives the analytical continuous source solution for dissolved radionuclide concentration in the borehole, C (in mg/L), as a function of time, t, and distance, x, from the source.

$$C(x,t)=\frac{C_0}{2}e^{\frac{x}{2\alpha_x}\left[1-\left(1+\frac{4\lambda\alpha_x}{v_c}\right)^{1/2}\right]}erfc\left(\frac{x-v_c t\left(1+\frac{4\lambda\alpha_x}{v_c}\right)^{1/2}}{2\left(\alpha_x v_c t\right)^{1/2}}\right) \qquad \text{Eq. 3.4-1}$$

where:

$$v_c = v / R_f \qquad \text{Eq. 3.4-2}$$

$$R_f = 1 + (\rho_b\, k_d) / n \qquad \text{Eq. 3.4-3}$$

and:

C_o = initial source concentration (mg/L)

v_c = dissolved radionuclide velocity (m/yr)

v = hydrologic pore velocity (m/yr)

R_f = retardation factor

k_d = distribution coefficient (L/g)

n = porosity of sealed borehole

ρ_b = bulk density of sealed borehole (kg/m^3)

α_x = longitudinal dispersivity (m)

λ = decay constant (yr^{-1})

Inputs used in the confidence-building exercise and assumptions made include:

- 400 PWR assemblies (~150 MT of heavy metal) vertically stacked down the length of the waste disposal zone (~ 2 km).
- Initial radionuclide inventory of iodine consistent with Brady et al. (2009, Appendix A). Effects of ingrowth accounted for in a bounding fashion.
- Solubility limits of dissolved radionuclides (Brady et al. 2009, Table 4).

- A constant thermally driven hydrologic flow from the top of the waste disposal zone upward through 1000 m seal zone with a vertical fluid velocity (specific discharge) of 0.017 m/yr for 200 yr (Brady et al. 2009, Figure 8).
- Pumping of borehole water from the top of the seal zone to the surface (biosphere) via a withdrawal well. No credit is taken for sorption or decay along the saturated zone transport pathway from the borehole to the withdrawal well in this benchmark exercise.
- A dilution factor of 3.16×10^7 (Brady et al. 2009, Section 3.2.3) is applied to account for the fact that the borehole water would mix with water in an existing aquifer before it would be captured by the withdrawal well (assumed to supply 1,000 people).
- Doses to a hypothetical person living near the withdrawal well are based on biosphere dose conversion factors consistent with the lifestyle of the Yucca Mountain reasonably maximally exposed individual, as specified by the Environmental Protection Agency (EPA) in 40 CFR 197 (EPA 2008).

The analytical solution determination of the source concentration at the top of the waste disposal zone is explained in (Brady et al. 2009, Section 5). The deep borehole GDS model simulates transport both in the waste disposal and seal zones. However, for comparison to the analytical solution results of only transport in the seal zone are needed. In this exercise several bounding and conservative assumptions were made. These include: all waste is assumed to instantly degrade and dissolve inside the waste packages; all waste is assumed to be PWR assemblies; and no credit is taken for sorption or decay along the saturated zone transport pathway from the sealed borehole to the withdrawal well.

The analytical solution was implemented in an MS Excel spreadsheet. Both the analytical solution and the deep borehole GDS model were run out to 200-yr simulation time. The concentration results for ^{129}I at the top of the seal zone as a function of time are shown in Figure 3.4-4. The results of the two methods are very close. The simulated concentrations at the top of the seal zone at 200 yr for the analytical solution and deep borehole GDS model are 9.71×10^{-8} mg/L and 9.91×10^{-8} mg/L, respectively. The results of the analytical solution presented here are slightly different from those reported in Brady et al. (2009, Table 6). In Brady et al. (2009, Table 6) a one-term analytical solution was used for simplicity, while for this exercise a two-term analytical solution was used. These results show that the deep borehole GDS model provides reasonably accurate simulation results for transport of radionuclides from the borehole to the accessible environment.

3.4.2.2 Model Demonstration

This subsection discusses the demonstration of capability for the current deep borehole GDS model. The results are presented in terms of the mean radionuclide mass release rates from the three major system components (i.e., disposal zone, seal zone and upper zone) as the intermediate result, and the mean dose (mrem/yr) by individual radionuclides at the hypothetical accessible environment which is assumed to be located on the surface, directly above the deep borehole. Note that the deep borehole modeling is an on-going effort, and improvements including incorporation of a more fundamental description of the disposal process will be made as information from other UFD work packages matures and becomes available. These improvements will be made directly into the GPAM in the future. Use of the mean dose is an arbitrary choice to present and discuss the analysis results in order to facilitate studies among the GDS options and does not indicate any realistic dose implications. Therefore, the results presented in this section for the model capability demonstration *should not* be construed as being indicative of the true performance of a deep borehole system or compared to any regulatory performance objectives regarding repository performance.

The model demonstration analysis was performed probabilistically, with 100 realizations for each modeling case and for a time period of 1,000,000 yr.

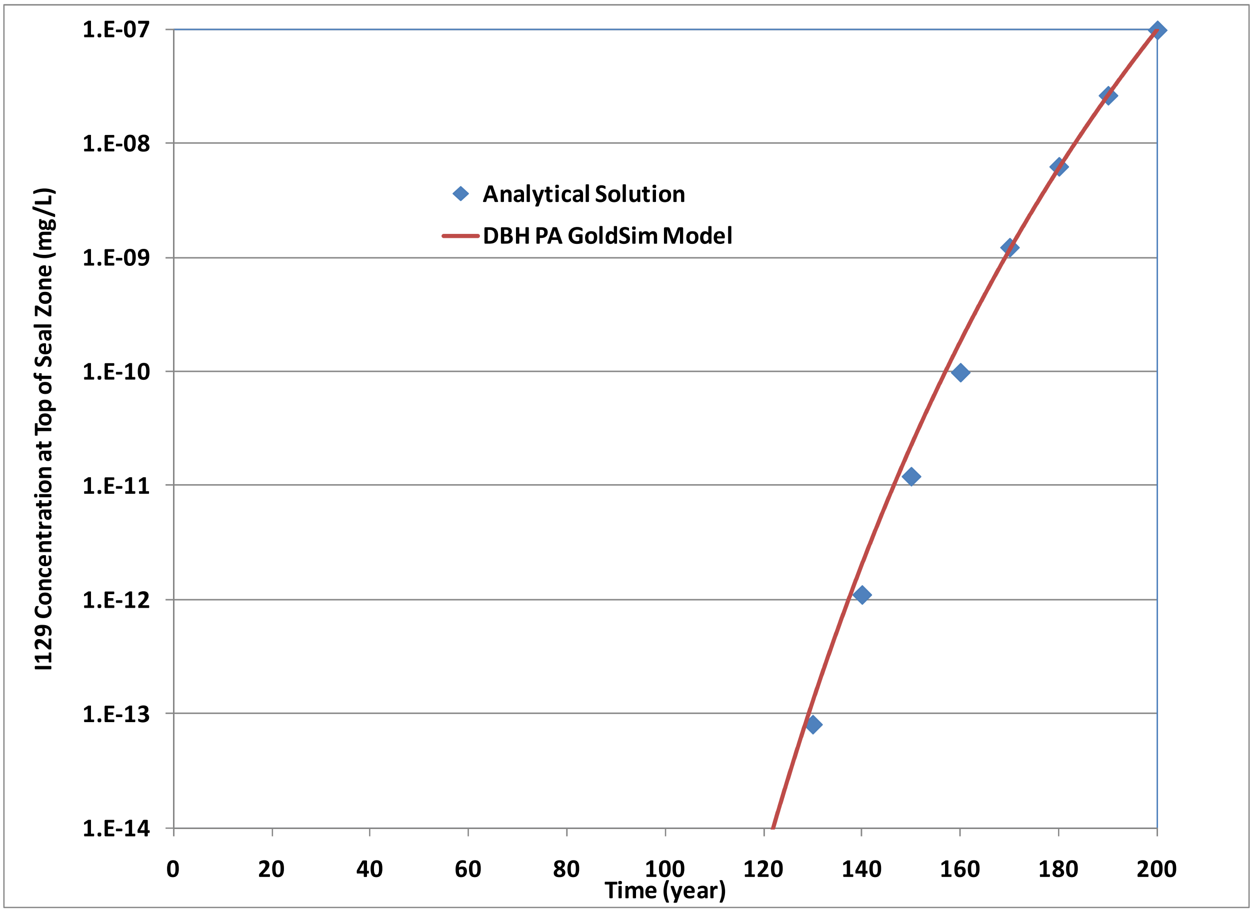


Figure 3.4-4. Comparison of ^{129}I Concentration Predictions at Top of Seal Zone for the Analytical Solution and Deep Borehole GDS Model

3.4.2.2.1 Base Permeability Case

This subsection analyzes the demonstration results for the base permeability case (Table 3.4-2). The base permeability case represents the expected permeability of geologic materials that comprises the deep borehole system and is the reference case. Two different waste inventory cases were analyzed: (1) 400 waste packages of commercial UNF, each containing a single PWR assembly, and (2) 400 waste packages of DHLW, each containing a single borosilicate glass canister.

Commercial UNF Inventory

Figure 3.4-5 shows the upward volumetric water flow rate histories at different locations in the disposal and seal zones for the base permeability case for the disposal of the commercial UNF inventory. The flow rate histories were obtained from detailed thermal hydrologic process-level analysis results and input to the deep borehole GDS model as a look-up table. The volumetric flow rate is for a borehole with the cross-sectional area of 1 m^2. In some instances the flow rates at certain locations and times could be downward directed. For all downward flow rates from the thermal-hydrologic analysis, a very small value has been assigned for conservatism and model simplification. The simplifications will be removed in the future. The outcome of the adjustment is shown as vertical curves leading to the very small value off the scale of y-axis. For the location and time period corresponding to the arbitrary small value, upward advective water flows are negligibly small, and diffusion is the dominant mechanism to transport dissolved radionuclides in the disposal and seal zones.

Figure 3.4-6 shows results for the mean advective and diffusive radionuclide mass release rates from the disposal zone (i.e., top of the disposal zone). The waste inventory is assumed to be uniformly distributed along the length of disposal zone (i.e., 2,000 m). For most radionuclides the mean advective release rates are higher than the mean diffusive release rates at early times, but the mean diffusive release rates increase with time, exceeding the mean advective release rates in the later time periods. ^{129}I has the highest mean release rate by both transport mechanisms for the entire analysis time period.

Figure 3.4-7 shows the mean diffusive mass release rate from the seal zone (i.e., at the top of seal zone). Because of very low upwards water flow rate (especially near the top of seal zone for later time periods) and retardation by sorption, calculated mean advective release rates are negligibly small and not shown in the figure. The mean diffusive release rates are also very low due mainly to sorption on compacted bentonite used in the seal zone. Again, ^{129}I is the dominant radionuclide in terms of the mean mass release rate.

The impact of radionuclide retardation in the seal zone is shown for the very low mass release rates from the upper zone as shown in Figure 3.4-8. As discussed previously, a constant upward volumetric water flow rate of 2.35×10^{-3} m^3/yr is used for the upper zone for the entire analysis time period. The upper zone mean release rate for the nonsorbing radionuclides (^{129}I and ^{36}Cl) are about the same as the seal zone mean release rate; the upper zone mean release rate of ^{99}Tc is further reduced as it sorbs on the upper zone geologic materials.

Figure 3.4-9 shows the mean dose by individual radionuclides at the hypothetical accessible environment. ^{129}I is the dominant dose contributor, but the calculated radionuclide mean doses are negligibly small.

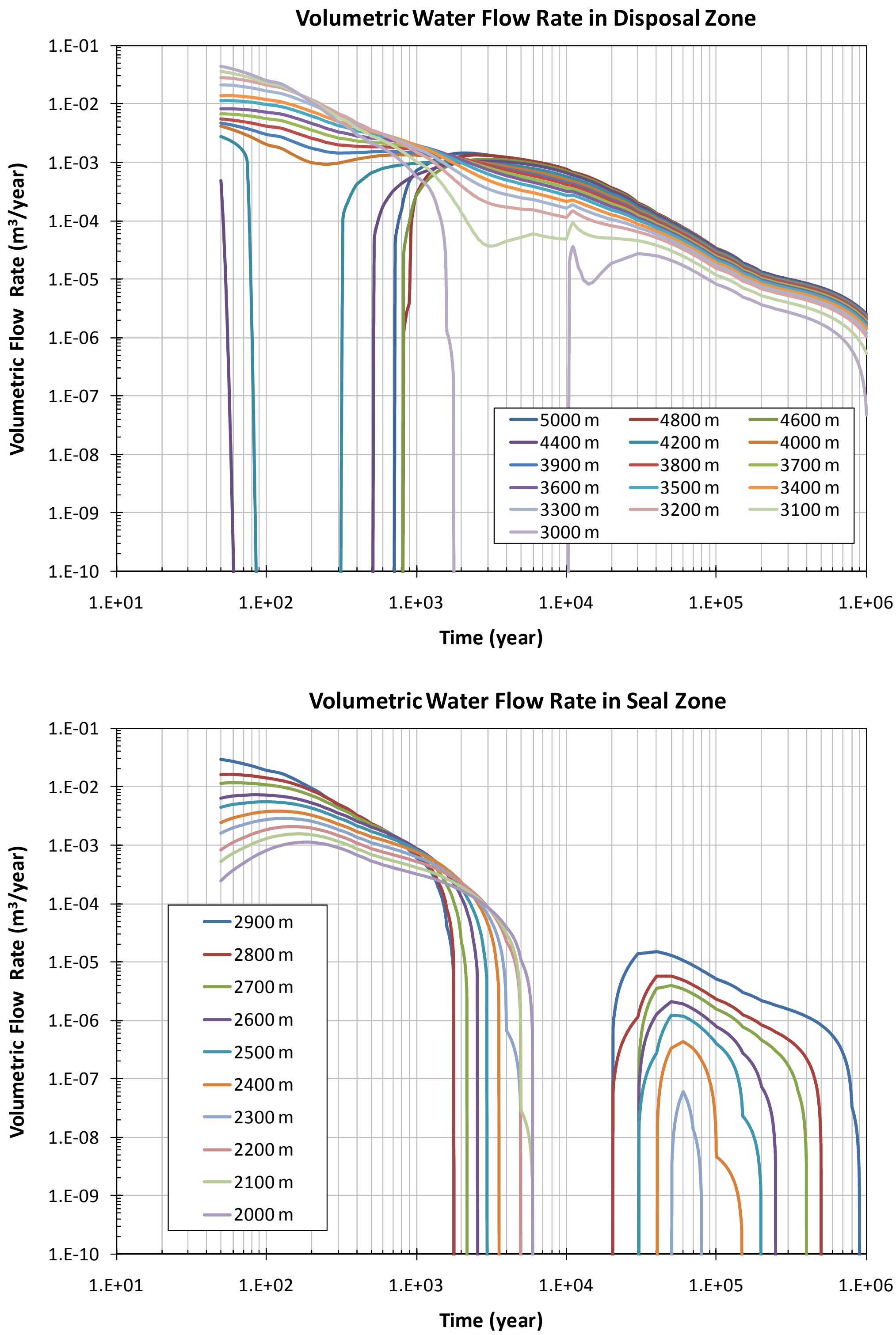
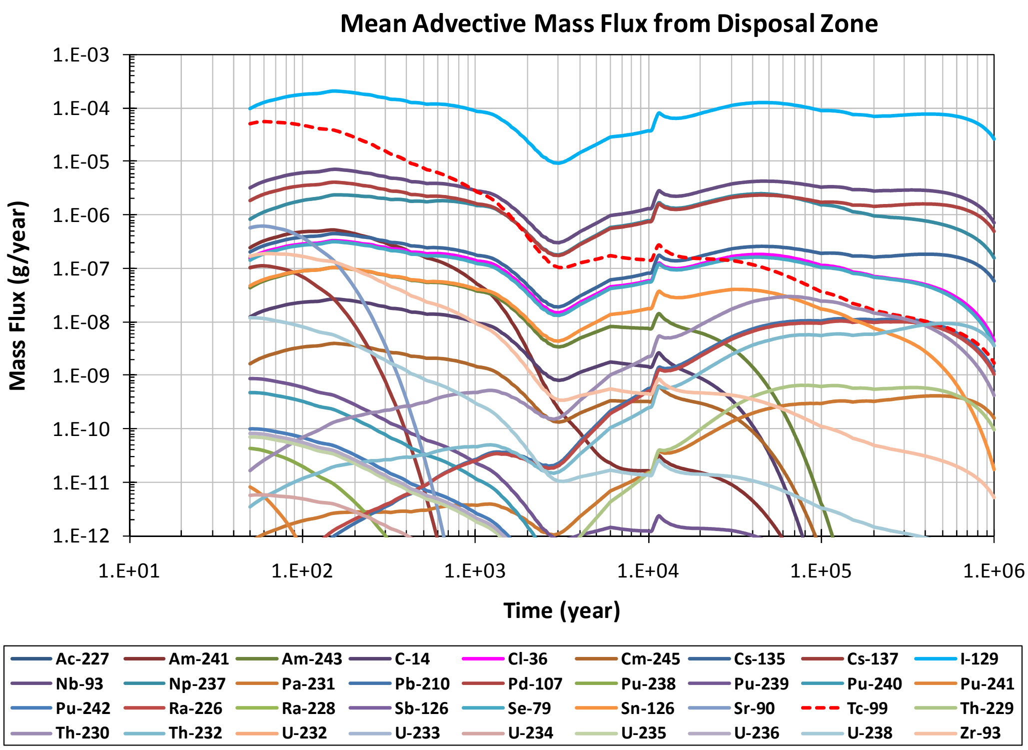


Figure 3.4-5. Volumetric Water Flow Rate Histories at Different Locations in the Disposal and Seal Zones for the Base Permeability Case: Commercial UNF



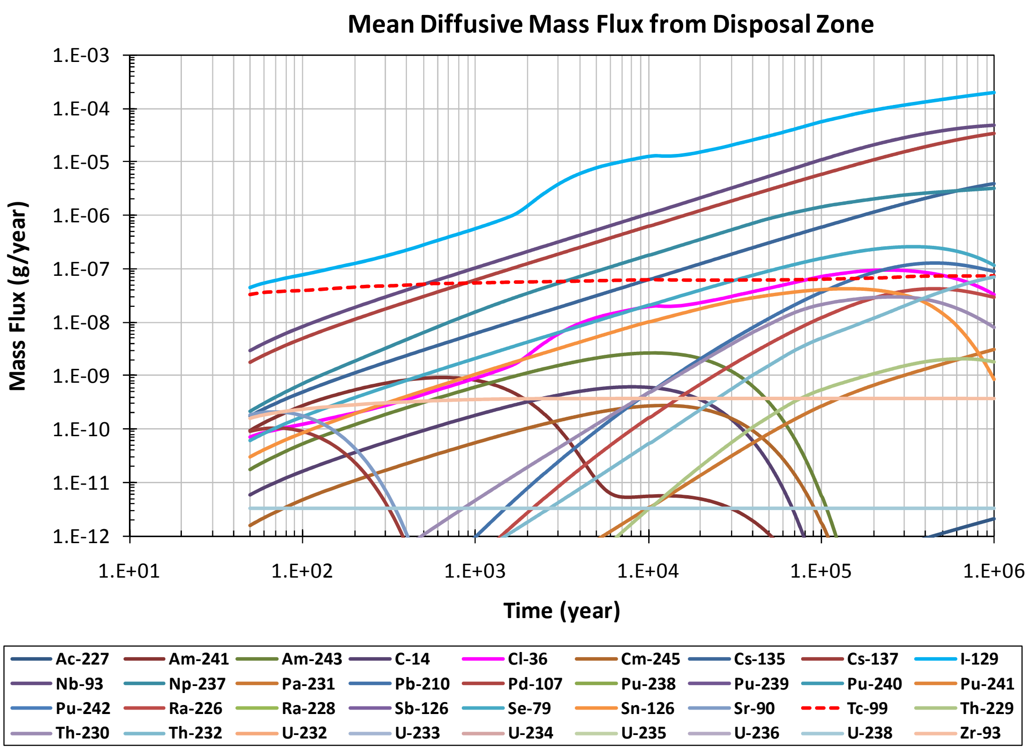
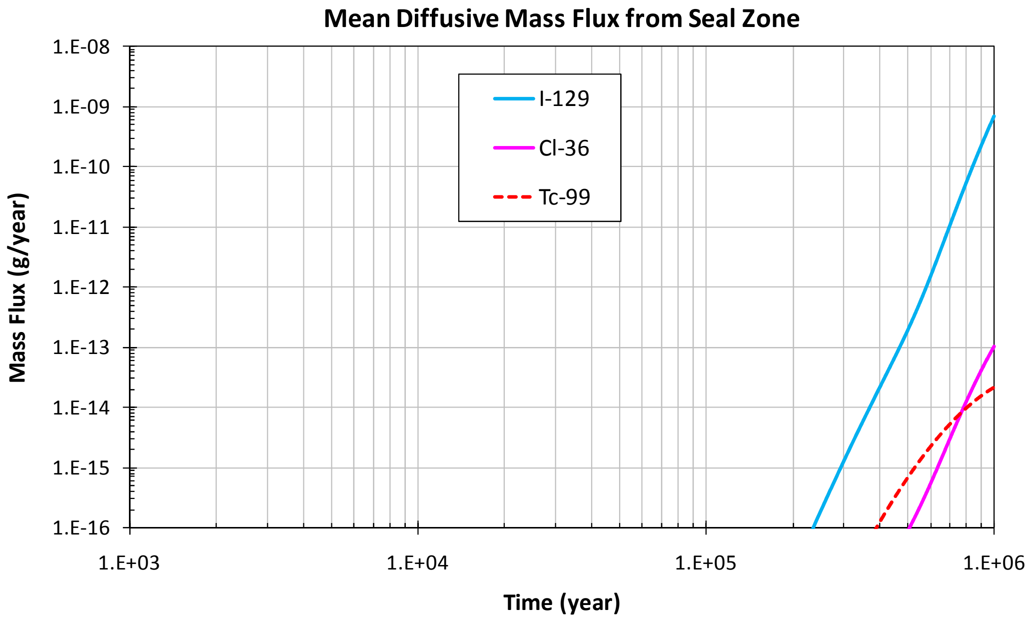


Figure 3.4-6. Commercial UNF Model Results for the Base Permeability Case: Mean Advective and Diffusive Mass Release Rate from Disposal Zone



NOTE: Advective mass release plot is not shown because of negligibly small release rate.

Figure 3.4-7. Commercial UNF Model Results for the Base Permeability Case: Mean Diffusive Mass Release Rate from Seal Zone

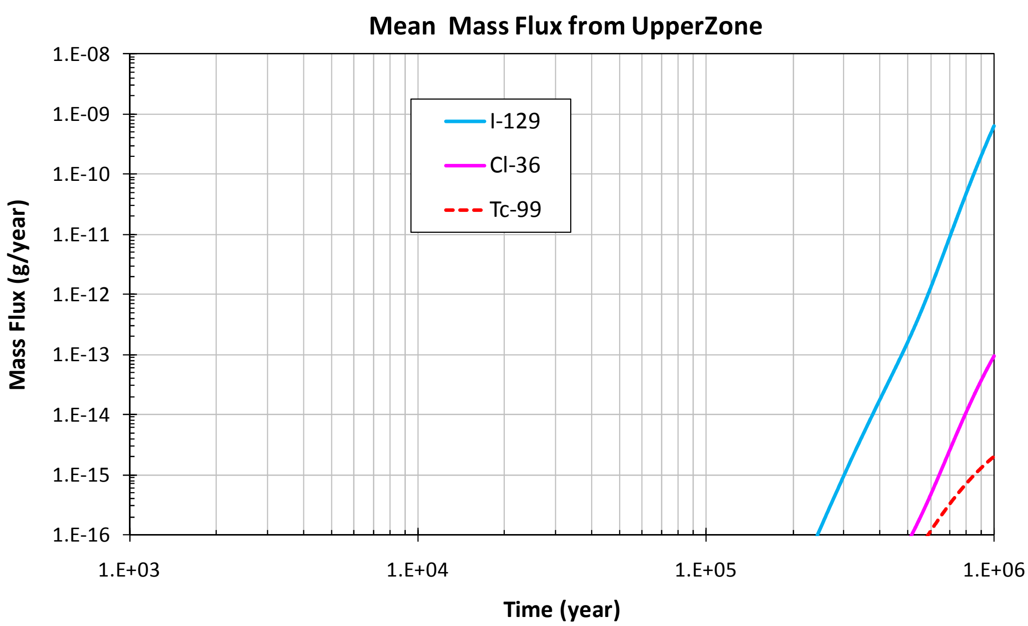


Figure 3.4-8. Commercial UNF Model Results for the Base Permeability Case: Mean Mass Release Rate from Upper Zone

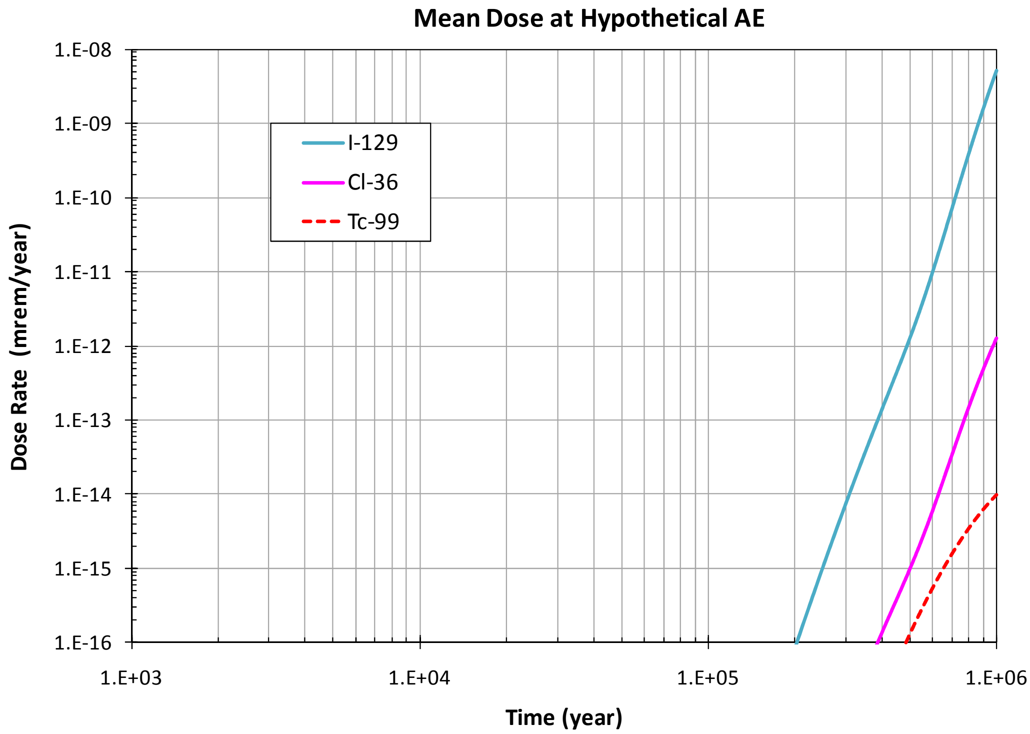


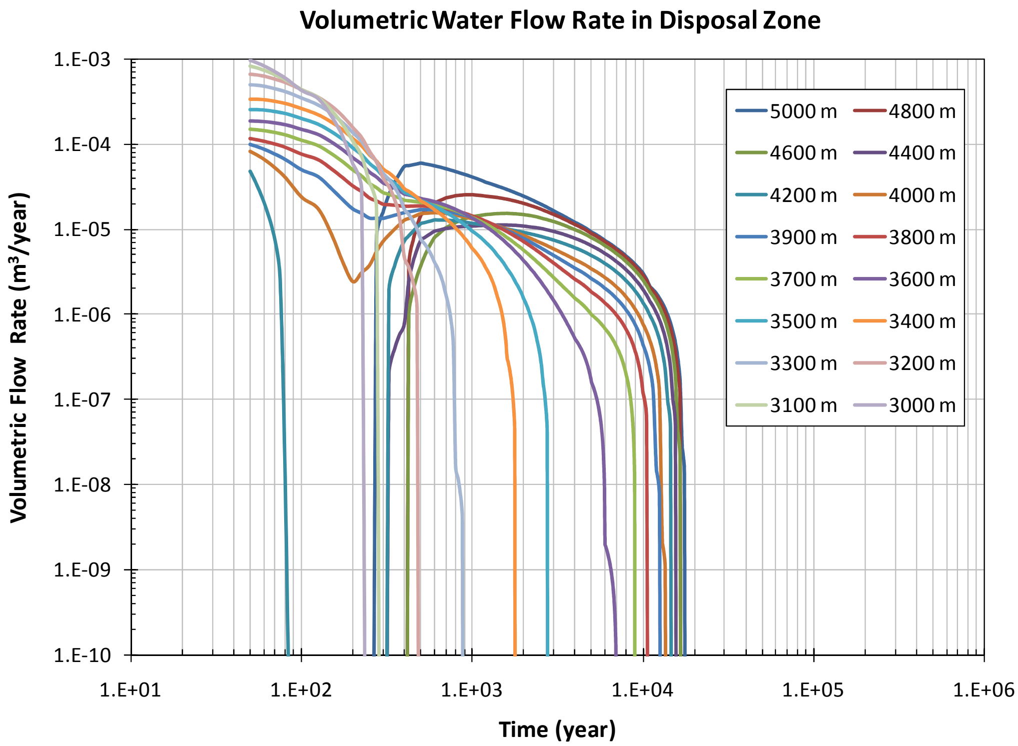
Figure 3.4-9. Commercial UNF Model Results for the Base Permeability Case: Mean Annual Dose at the Hypothetical Accessible Environment Located above the Repository

DHLW Inventory

Figure 3.4-10 shows the results of the DHLW inventory for the upward volumetric water flow rate histories at different locations in the disposal and seal zones for the base permeability case. The flow rate histories are different from those for the commercial UNF inventory for the same base case permeability case because of the different decay heat output characteristics between the two waste types. For the disposal zone, no upward water flows exist at all after about 20,000 yr, and upward water flows stop at about 300 yr near the upper portion of the zone (at depths of 3,000 and 3,100 m). In the seal zone no upward flows exist after about 2,000 yr. The lack of upward water flows has significant impact on the radionuclide transport, and slow diffusion processes will be the dominant transport mechanism to move dissolved radionuclides toward the hypothetical accessible environment located at the surface.

Impact of the lack of upward water flows is shown for the mean advective release rate from the disposal zone in Figure 3.4-11, which shows cessation of advective transport from the disposal zone at about 300 yr; this corresponds to the cessation of the upward flows at the top of disposal zone. The diffusive release rates are still noticeable, and the ^{129}I mean release rate reaches a broad maximum of about 10^{-3} g/yr between 3,000 and 6,000 yr.

Figure 3.4-12 shows the mean diffusive release rate from the seal zone, and only ^{129}I has noticeable release rates. Again advective releases are not shown because of negligibly small values. The upper zone mean release rate of ^{129}I (nonsorbing) shows a similar behavior to the seal zone release rate. As shown in Figure 3.4-13, ^{129}I is the only dose-contributing radionuclide at the hypothetical accessible environment, and the calculated mean doses are negligibly small.



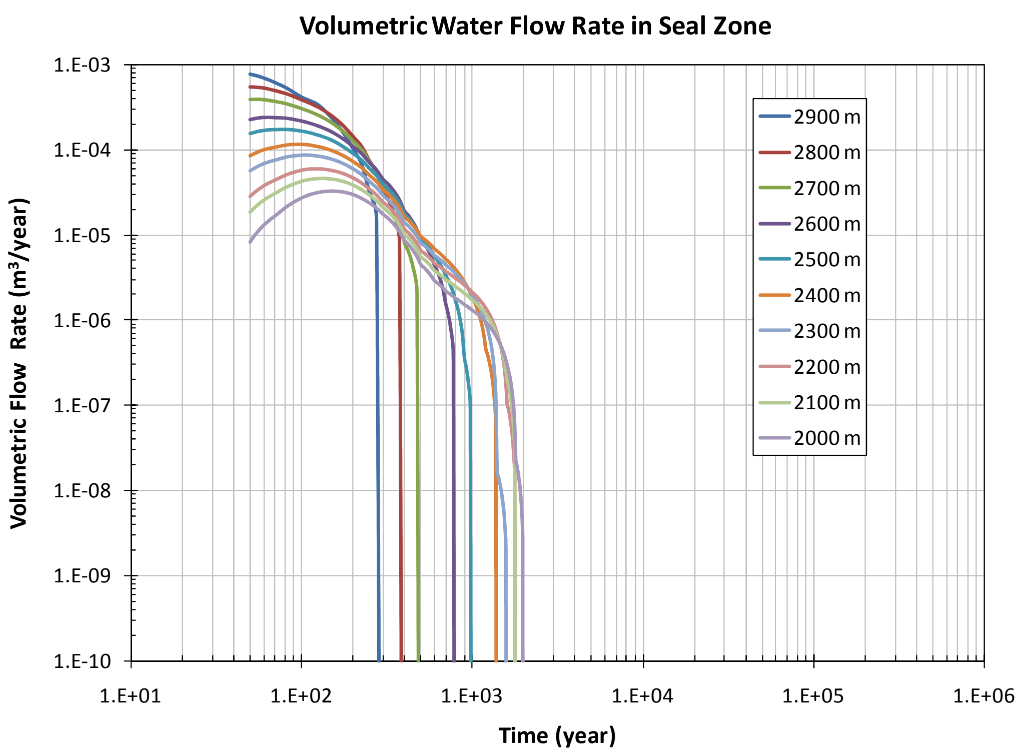


Figure 3.4-10. Volumetric Water Flow Rate Histories at Different Locations in the Disposal and Seal Zones for the Base Permeability Case: DHLW

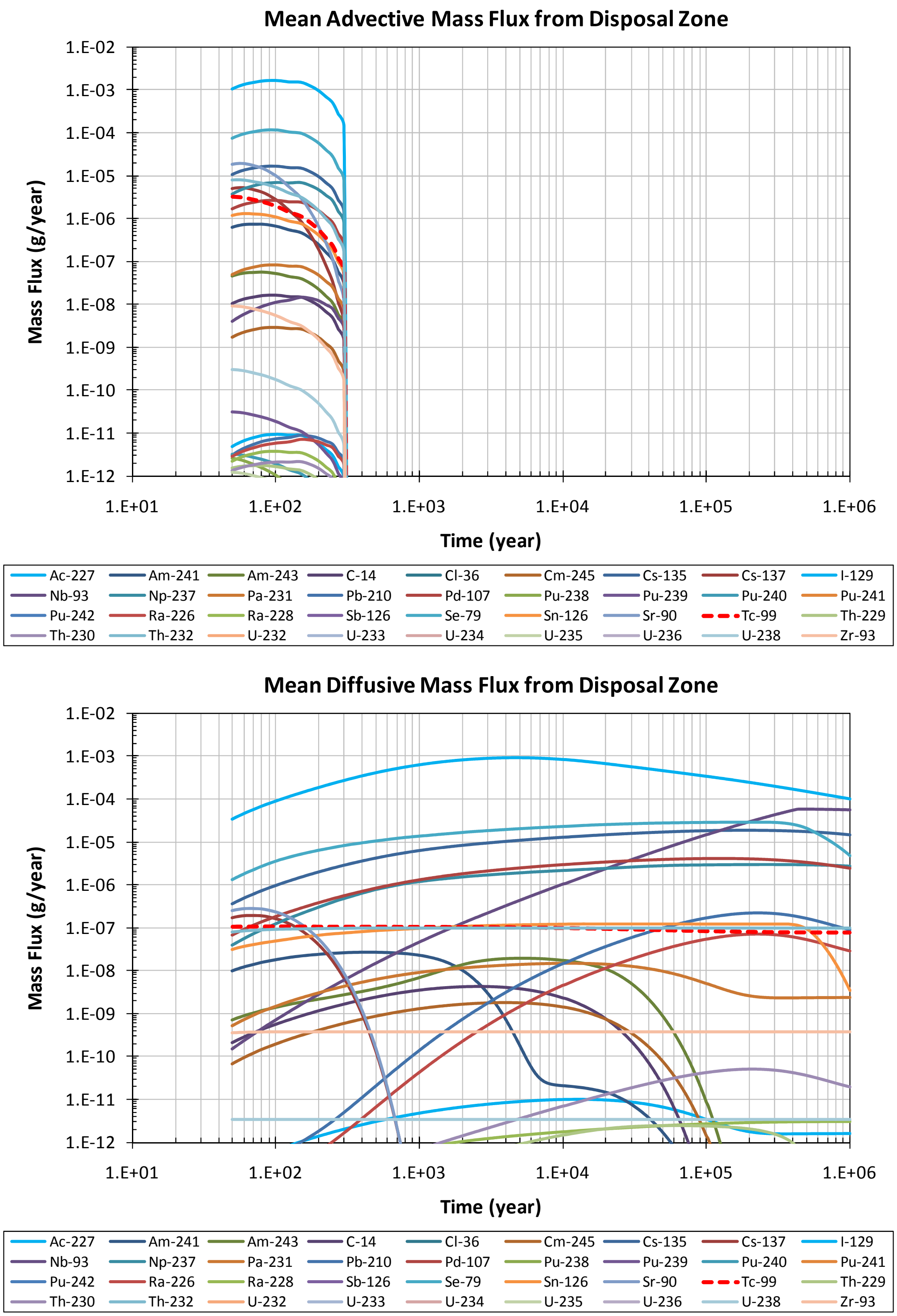
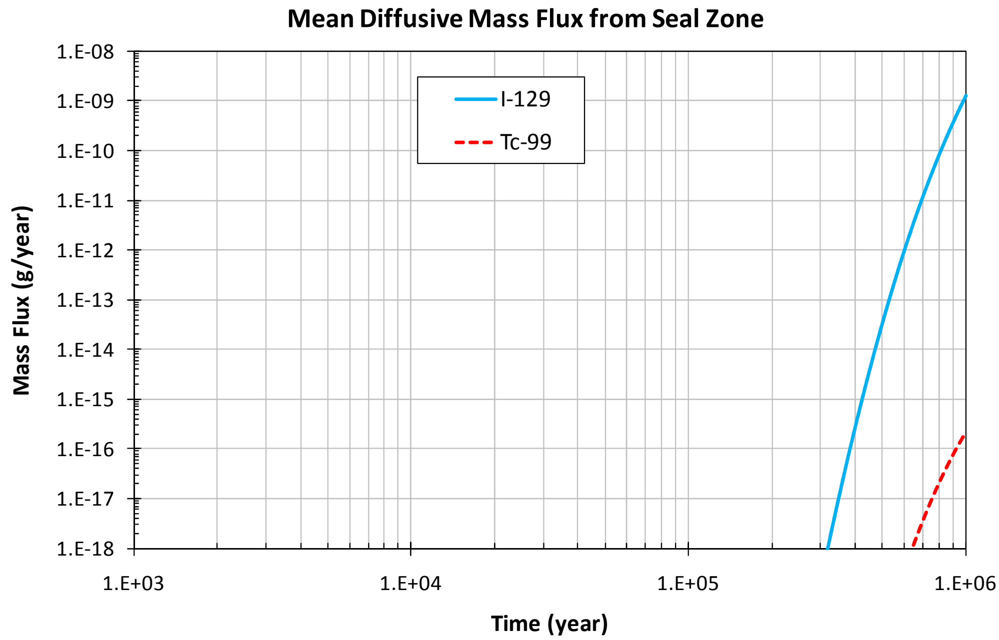


Figure 3.4-11. DHLW Model Results for the Base Permeability Case: Mean Advective and Diffusive Mass Release Rate from Disposal Zone



NOTE: Advective mass release plot is not shown because of negligibly small release rate.

Figure 3.4-12. DHLW Model Results for the Base Permeability Case: Mean Diffusive Mass Release Rate from Seal Zone

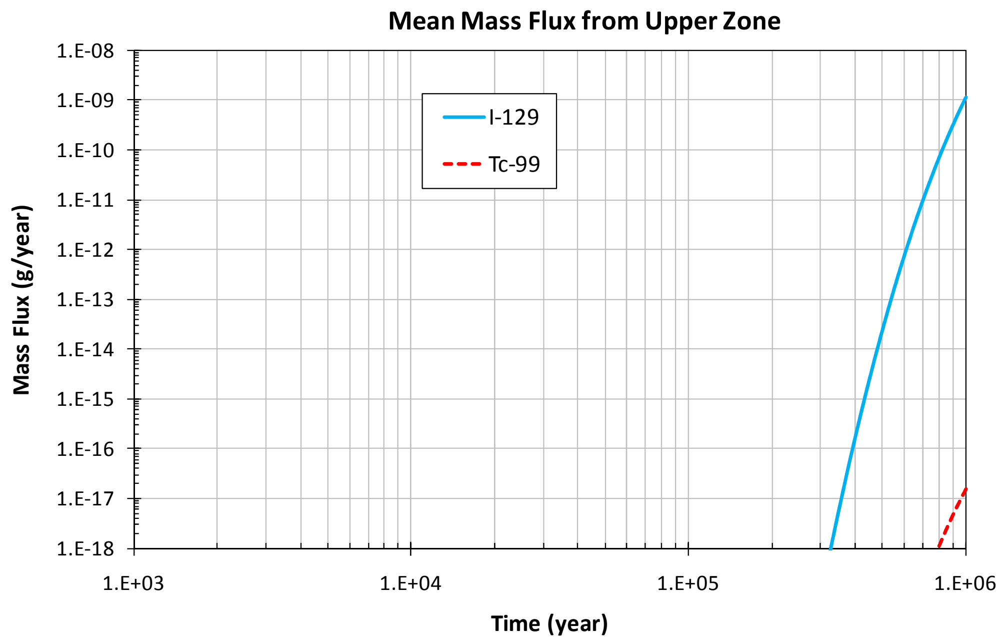


Figure 3.4-13. DHLW Model Results for the Base Permeability Case: Mean Mass Release Rate from Upper Zone

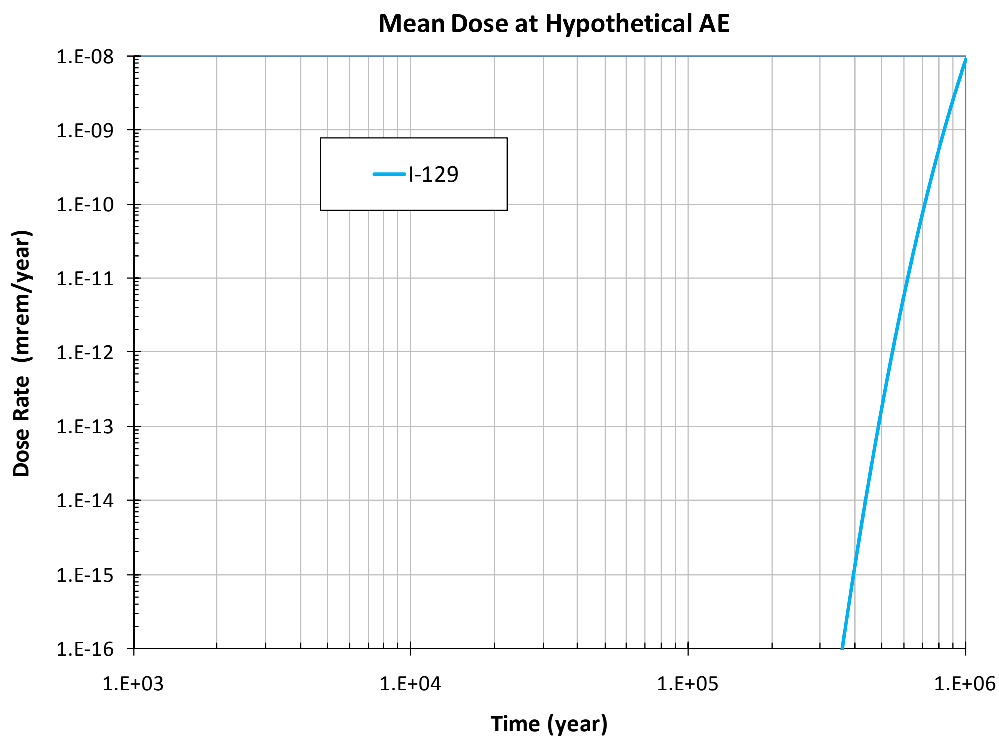


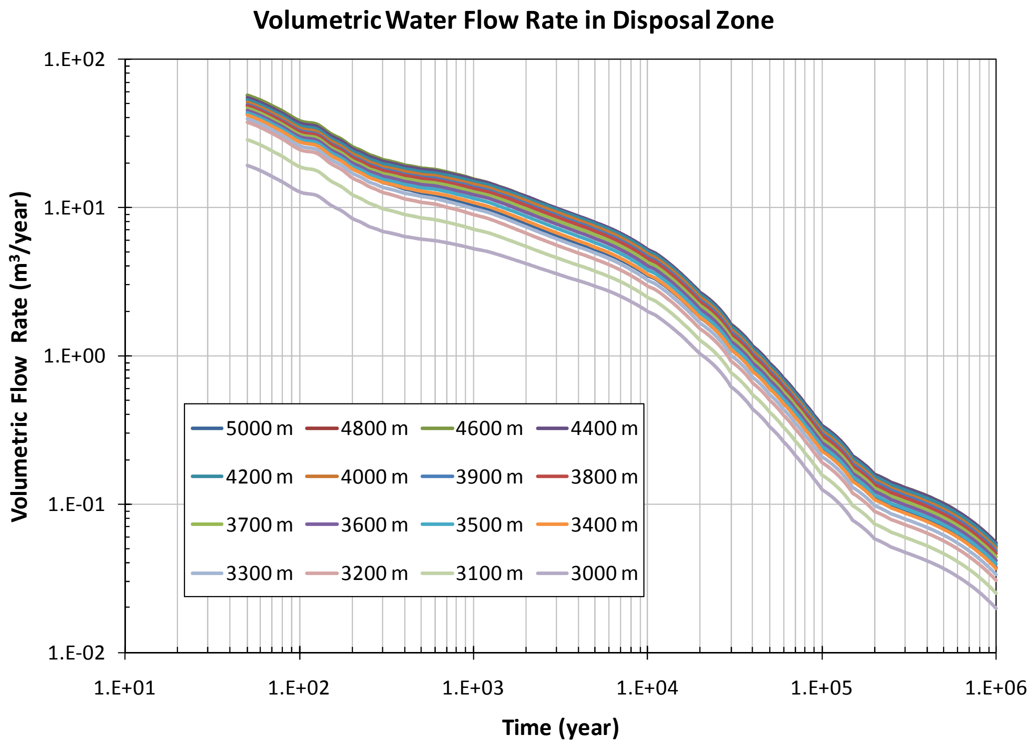
Figure 3.4-14. DHLW Model Results for the Base Permeability Case: Mean Annual Dose at the Hypothetical Accessible Environment Located above the Repository

3.4.2.2.2 High Permeability Case

Sensitivity analyses were conducted to evaluate an assumed condition with a much higher permeability for the system components than the base case permeability. The high permeability case represents a highly conservative bounding condition, for which the system components (e.g., host rock, disturbed rock zone, seals, etc.) have grossly failed, resulting in a much higher permeability than the expected design permeability values. Process-level thermal hydrology simulations were conducted with the assumed bounding permeability values (Table 3.4-2). This subsection analyzes the deep borehole GDS results for the high permeability case.

Commercial UNF Inventory

Figure 3.4-15 shows the results of the upward volumetric water flow rate histories at different locations in the deep borehole disposal and seal zones for the high permeability case disposing of commercial UNF inventory. As shown in the figure, upward water flows at considerably higher rates than the base permeability case for both zones over the entire simulation time. The same constant upward volumetric water flow rate of 2.35×10^{-3} m^3/yr used in the upper zone of the base case is also used in the upper zone for the high permeability case. The water flow profiles suggest that advective transport may be the dominant mechanism to move dissolved radionuclides upwards to the surface.



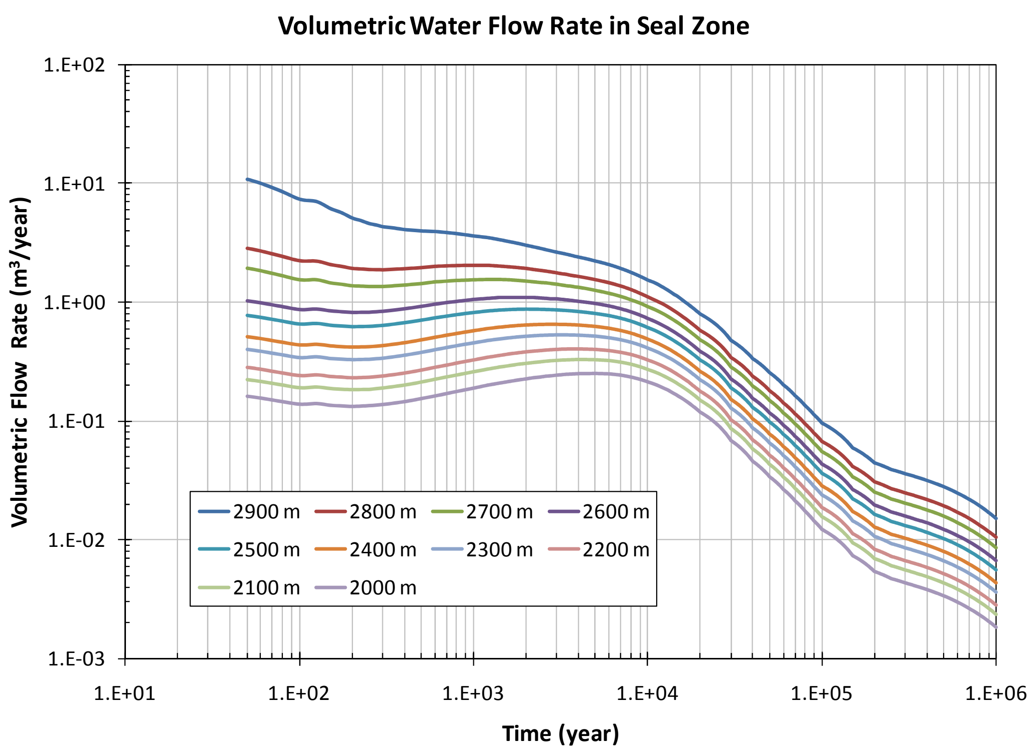


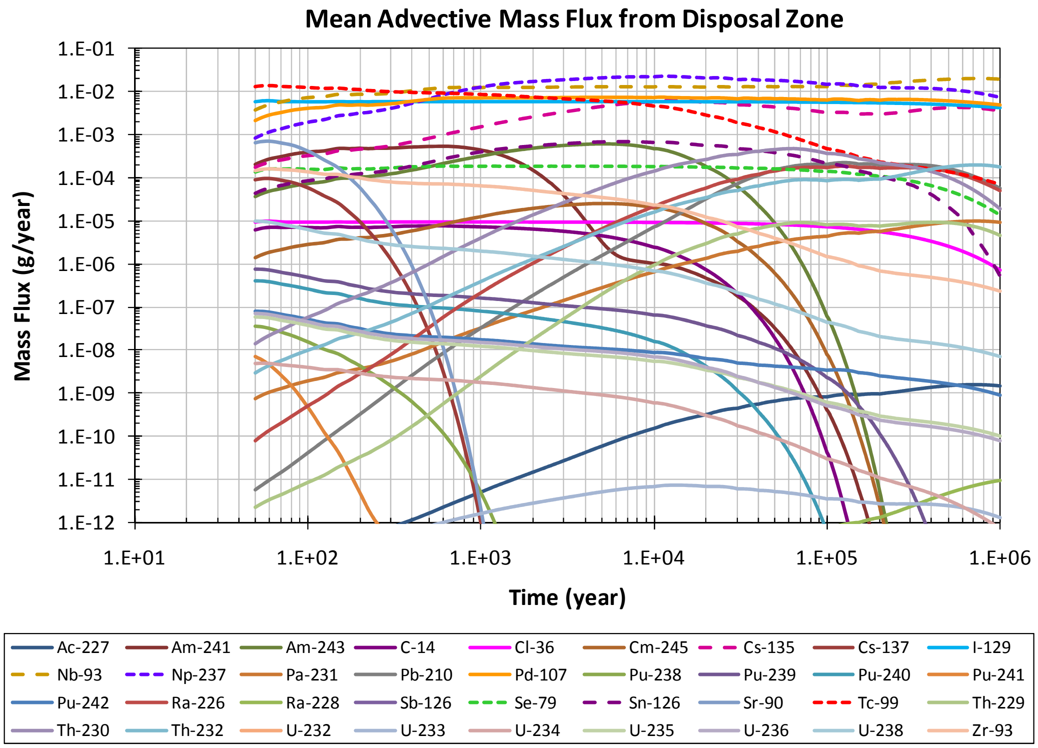
Figure 3.4-15. Volumetric Water Flow Rate Histories at Different Locations in the Disposal and Seal Zones for the High Permeability Case: Commercial UNF

Figure 3.4-16 shows the model results for the mean advective and diffusive radionuclide mass release rate from the disposal zone. The waste inventory is uniformly distributed along the length of disposal zone (2,000 m). As expected from the water flow rate profiles, the mean advective release rates are much higher than the mean diffusive release rates for the entire simulation time period. For advective transport in the disposal zone, other radionuclides such as ^{237}Np, ^{107}Pd and ^{93}Nb have higher mean release rates than ^{129}I. Note that ^{129}I is not shown in the diffusive release figure, and this is because ^{129}I undergoes back-diffusion (i.e., negative diffusion or downward diffusive flux) for the entire analysis time period. The back-diffusion is caused by the large advective flux, which results in higher ^{129}I mass at a higher node than at a lower node. That causes downward diffusion. The advective component follows the direction of the vertical groundwater flux, which is upwards. The back-diffusion will be explored further in the future. ^{237}Np and ^{135}Cs are two dominant radionuclides in terms of the upwards diffusive release rates.

Figure 3.4-17 shows the mean advective and diffusive mass release rate from the seal zone (i.e., at the top of seal zone). ^{129}I has the highest mean release rate by both diffusion and advection, and the mean advective release rate is much higher than the mean diffusive release rate. The dominance of ^{129}I is due to the fact that no sorption has been assigned to it and also it has unlimited solubility. Compared to the base permeability case, many other radionuclides (notably ^{99}Tc, ^{36}Cl, ^{79}Se, etc.) are released at considerably high rates.

The mean mass release rates from the upper zone (Figure 3.4-18) show that ^{129}I is the dominant radionuclide and ^{99}Tc and ^{36}Cl are also important in terms of the peak mean release rate. A similar trend is shown for the mean dose at the hypothetical accessible environment, with ^{129}I being the dominant dose contributor (Figure 3.4-19). It is interesting to note that the dose contribution by ^{14}C is high relative to its peak mean mass release rate from the upper zone, and this is the outcome of mainly the high specific activity (4.47 Ci/yr) of the radionuclide.

The high permeability case is a highly conservative assumption. The results reinforce the importance of ensuring elimination of potential causes for high upward water flows in a deep borehole.



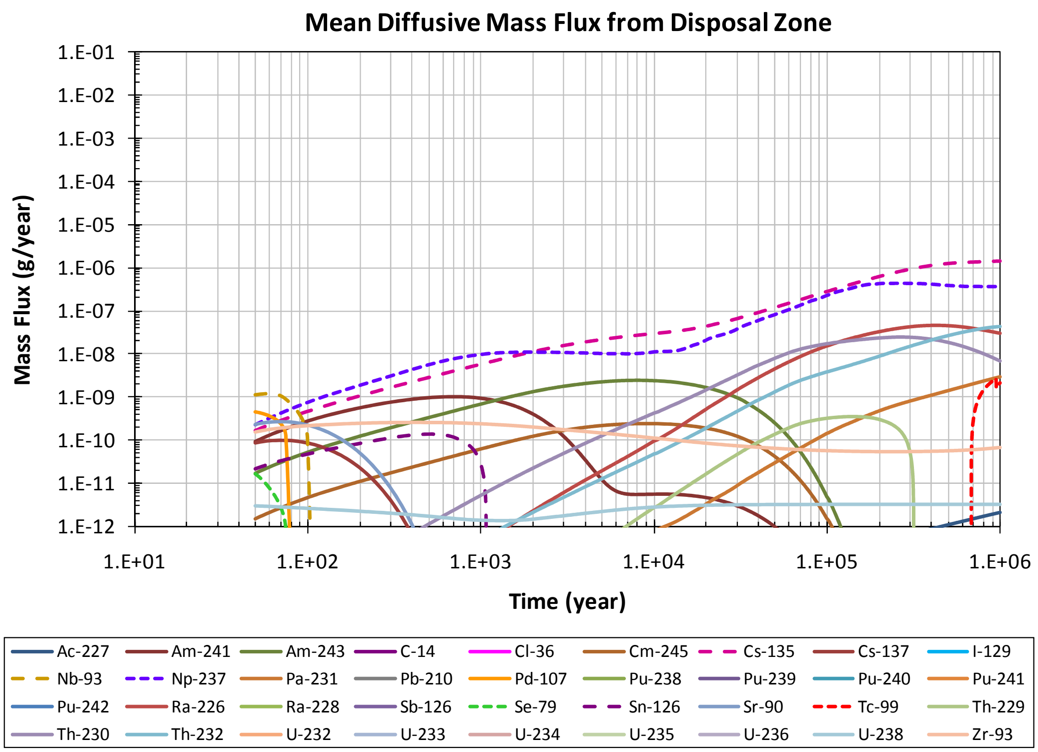
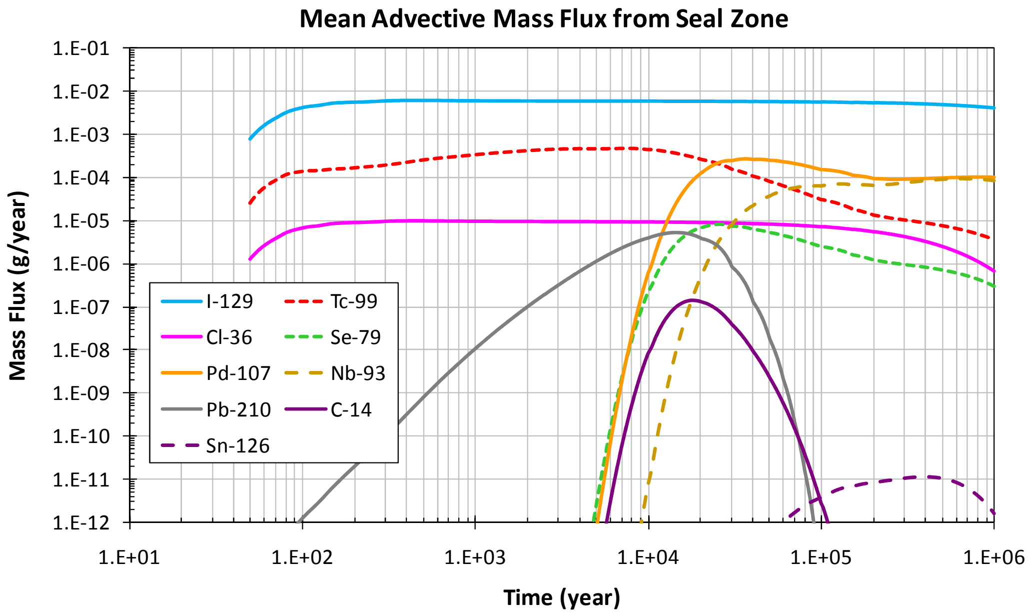


Figure 3.4-16. Commercial UNF Model Results for the High Permeability Case: Mean Advective and Diffusive Mass Release Rate from Disposal Zone



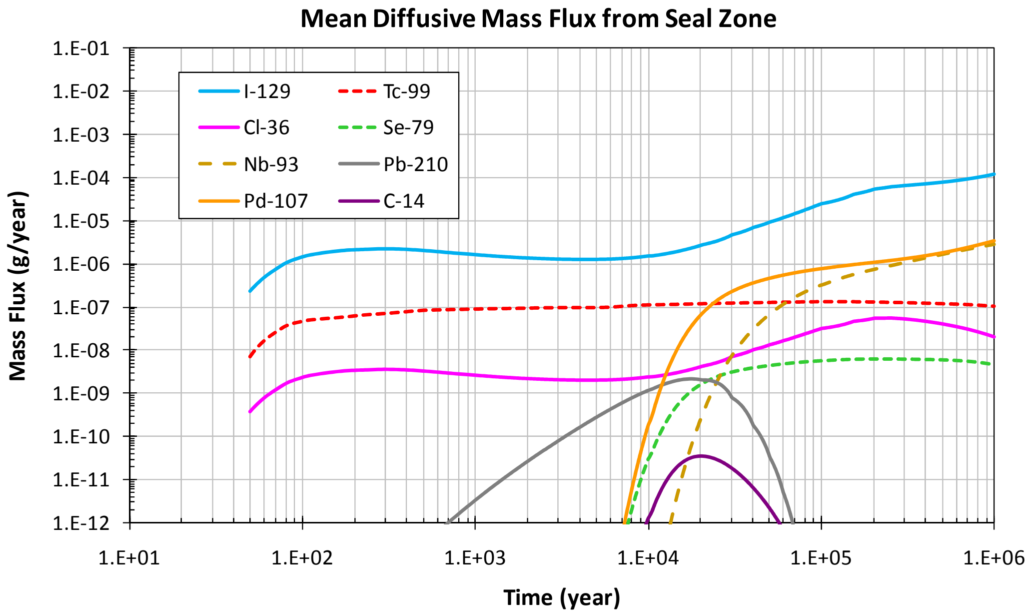


Figure 3.4-17. Commercial UNF Model Results for the High Permeability Case: Mean Advective and Diffusive Mass Release Rate from Seal Zone

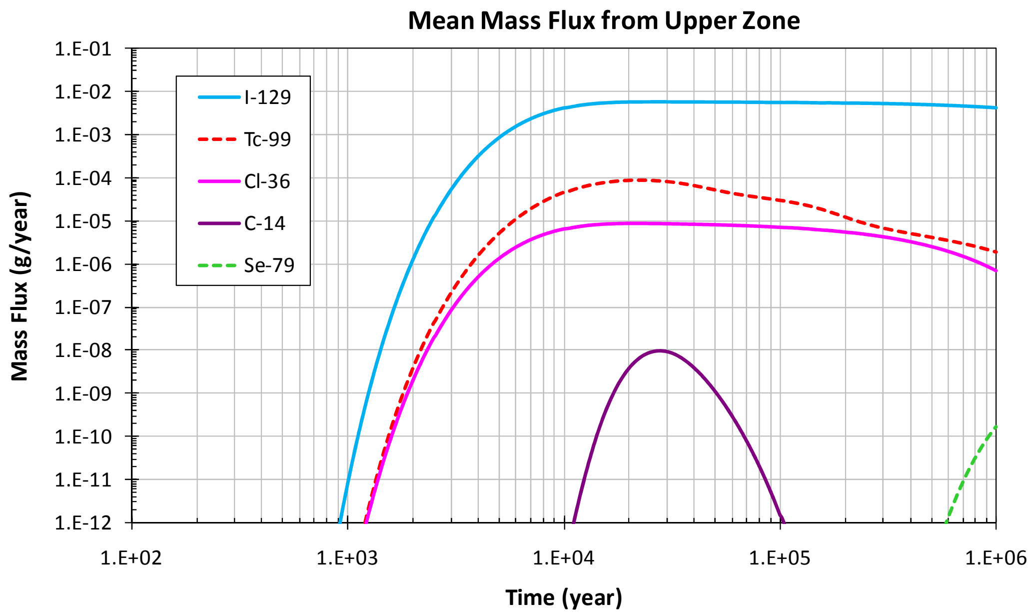


Figure 3.4-18. Commercial UNF Model Results for the High Permeability Case: Mean Mass Release Rate from Upper Zone

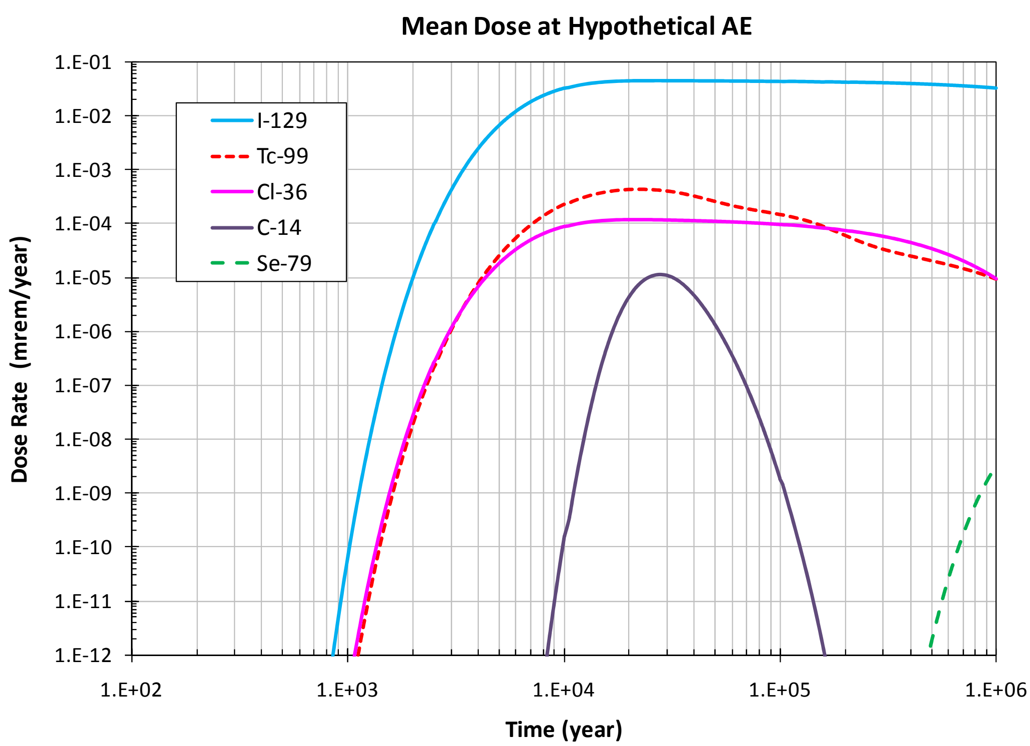


Figure 3.4-19. Commercial UNF Model Results for the High Permeability Case: Mean Annual Dose at the Hypothetical Accessible Environment Located above the Repository

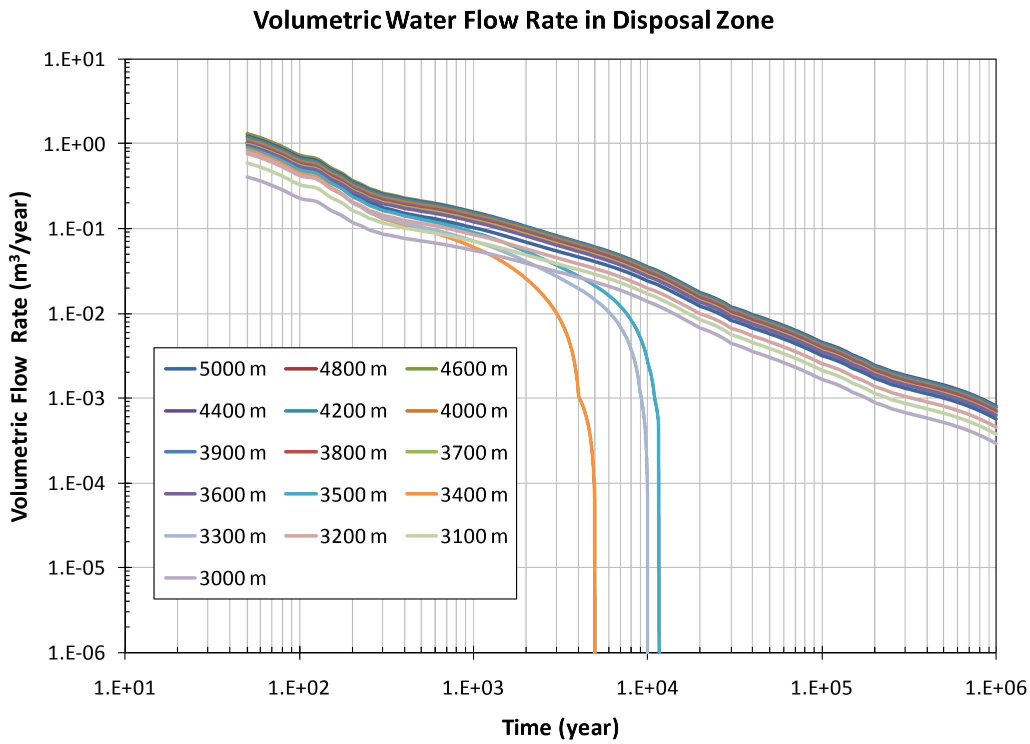
DHLW Inventory

For the DHLW inventory Figure 3.4-20 shows the upward volumetric water flow rate histories at different locations in the disposal and seal zones for the high permeability case. The upward flow rates are generally lower than the commercial UNF inventory case because of the lower heat loading. Some sections of the disposal zone (at depths between 3,500 and 3,300 m) have upward flows ceased after about 5,000 to 12,000 yr. The same constant upward volumetric water flow rate of 2.35×10^{-3} m^3/yr is also used for the upper zone for the entire analysis time period as was used in the other cases. As in the commercial UNF inventory case, advection will be seen to be the dominant transport.

Figure 3.4-21 shows the model results for the mean advective and diffusive radionuclide mass release rates from the disposal zone. As expected from the water flow rate profiles, the mean advective release rates are much higher than the mean diffusive release rates for the entire time periods. ^{129}I has the highest mean advective release rate until about 5,000 yr, then its release rates become comparable to the rates of other radionuclides (^{79}Se and ^{135}Cs). ^{129}I is not shown in the mean diffusive release rates figure because ^{129}I undergoes back-diffusion (i.e., negative diffusion or downward diffusive flux) for the entire analysis time period. The back-diffusion will be explored further in the future. ^{79}Se, ^{135}Cs and ^{93}Nb are also important radionuclides in terms of the diffusive release rates.

Figure 3.4-22 shows the mean advective and diffusive mass release rates from the seal zone. ^{129}I and ^{99}Tc are the only radionuclides that are released from the seal zone at significant rates, and all other radionuclides are greatly retarded in the seal zone mainly because of sorption on the bentonite seal material. ^{129}I is the single dominant radionuclide in terms of the mean release rates by both diffusion and advection, and the mean advective release rate is much higher than the mean diffusive release rate. It is interesting to note that the ^{129}I peak mean mass release rate is higher than that of the commercial UNF inventory case. This is a result of the higher degradation rate of the borosilicate glass waste form of the DHLW, which releases ^{129}I from the waste form at a faster rate. Both waste types have a comparable ^{129}I inventory.

The mean mass release rates from the upper zone (Figure 3.4-23) show a similar release behavior to that of the seal zone. The ^{129}I mean mass release rate reaches a peak at about 12,000 yr, and then decreases by about two orders of magnitude before it levels off. As stated above, the early peak is a caused by the higher degradation rate of the borosilicate glass waste form of the DHLW. It is also caused by the increased advection caused by the high permeability groundwater flux. As a result, the amount of ^{129}I in the system is depleted, causing the decreases in mass release rate at later times. The mean annual dose curves in Figure 3.4-24 also show a similar pattern to ^{129}I because they are dominated by ^{129}I. The magnitude of the ^{129}I peak mean annual dose is higher than that of the commercial UNF inventory case, reaching about 2 mrem/yr at 12,000 yr. The high permeability case is based on highly conservative assumptions, and the results reinforce the importance of ensuring elimination of potential causes for high upward water flows in a deep borehole.



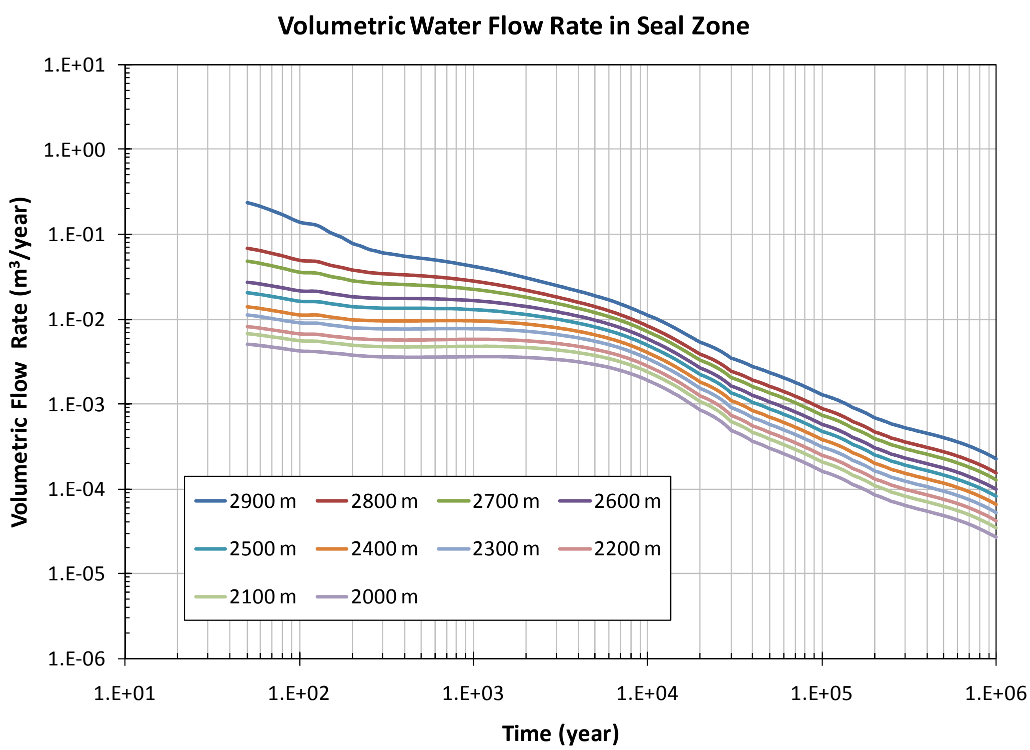
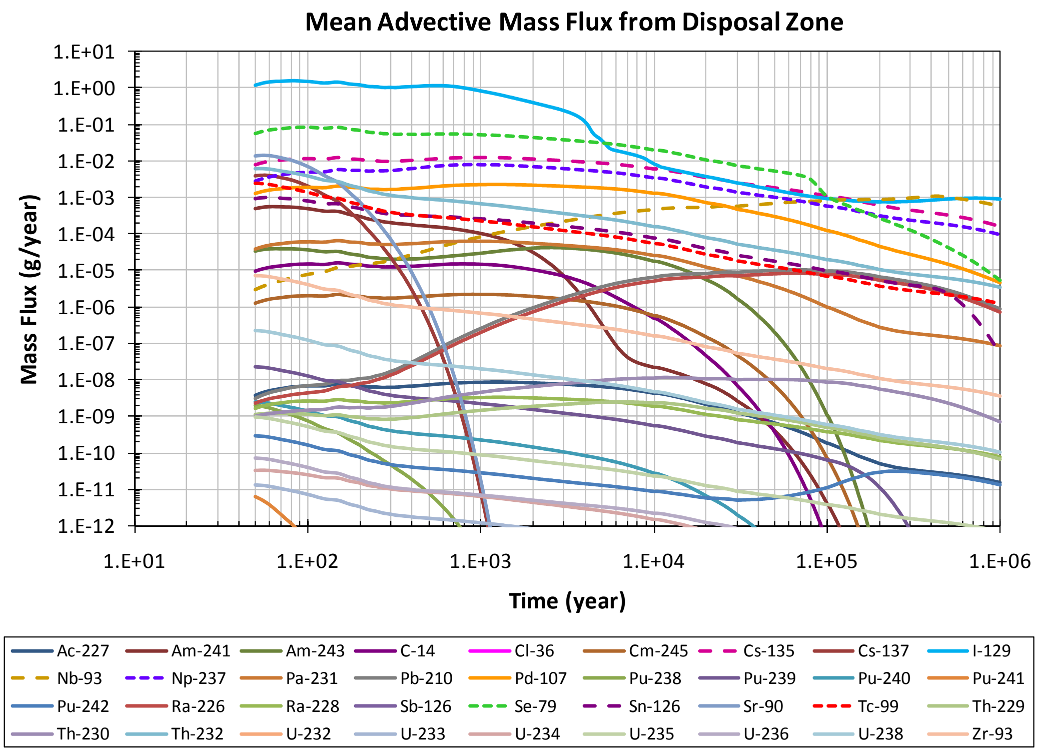


Figure 3.4-20. Volumetric Water Flow Rate Histories at Different Locations in the Disposal and Seal Zones for the High Permeability Case: DHLW



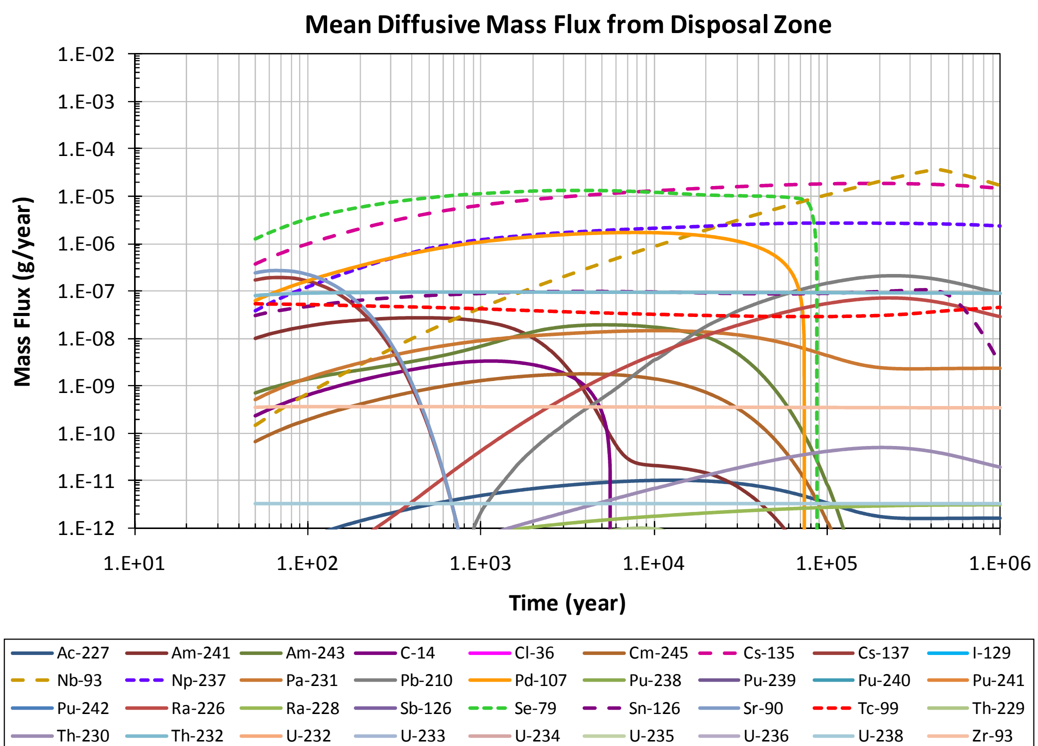
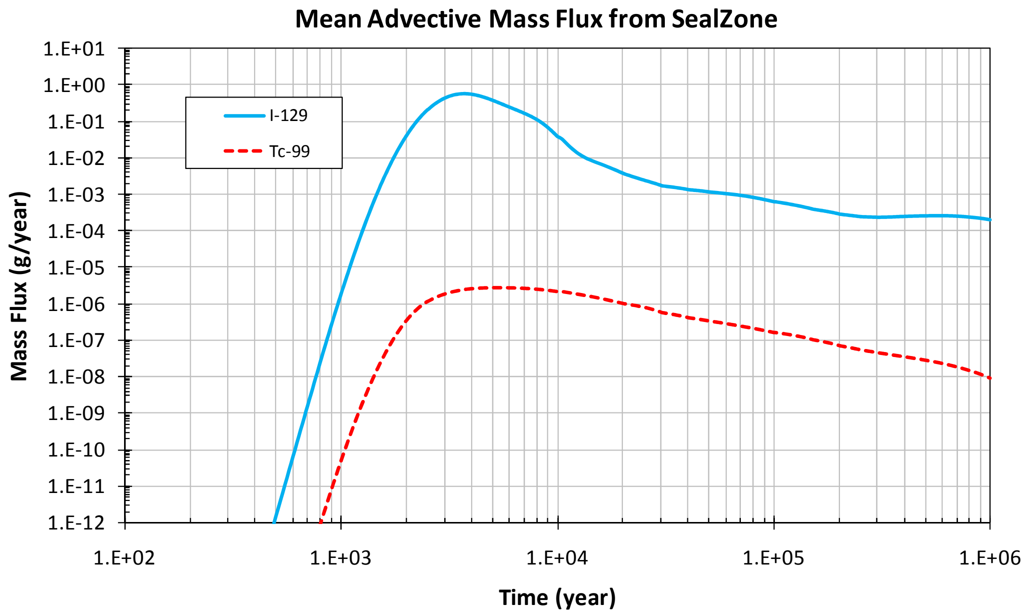


Figure 3.4-21. DHLW Model Results for the High Permeability Case: Mean Advective and Diffusive Mass Release Rate from Disposal Zone



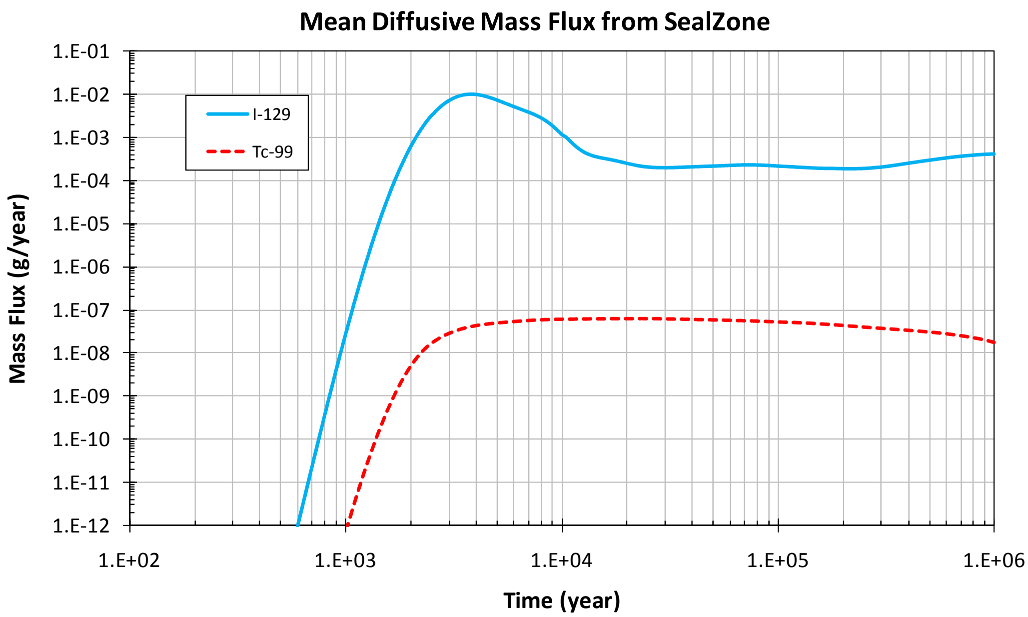


Figure 3.4-22. DHLW Model Results for the High Permeability Case: Mean Advective and Diffusive Mass Release Rate from Seal Zone

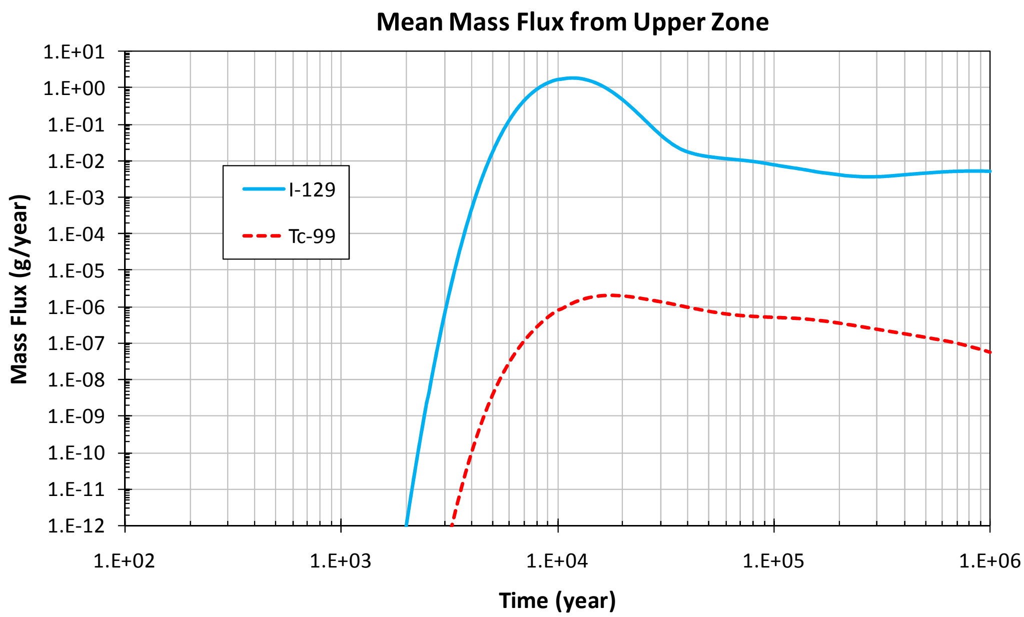


Figure 3.4-23. DHLW Model Results for the High Permeability Case: Mean Mass Release Rate from Upper Zone

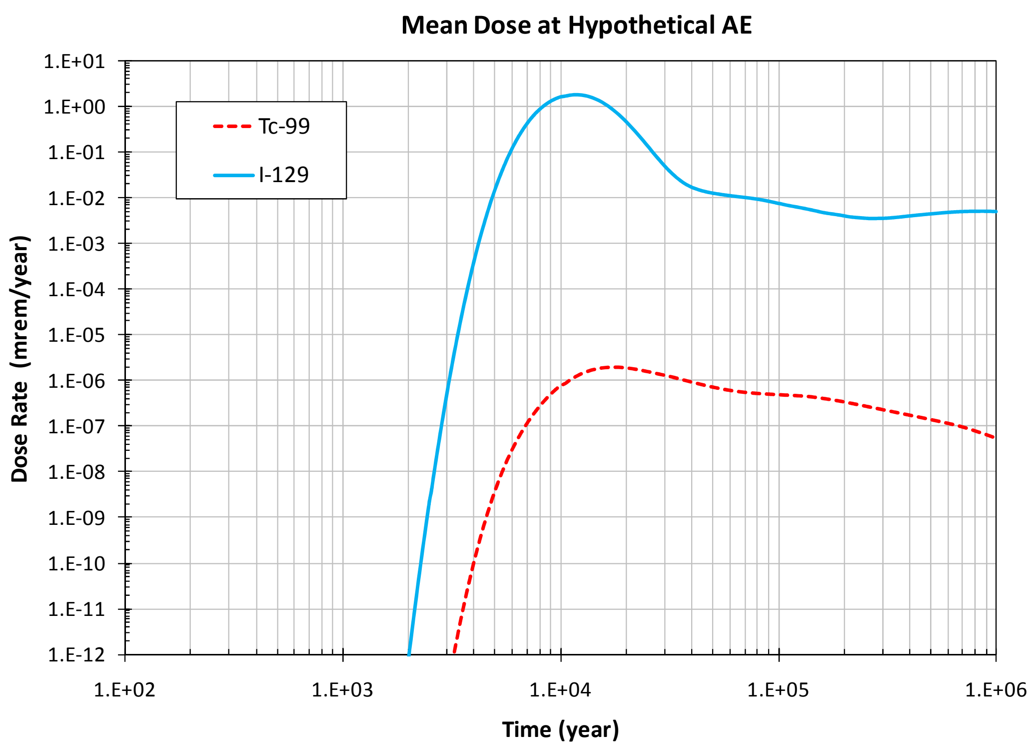


Figure 3.4-24. DHLW Model Results for the High Permeability Case: Mean Annual Dose at the Hypothetical Accessible Environment Located above the Repository

3.4.2.2.3 High Permeability Case with Iodine Sorbent (Getter) in the Seal Zone

The model analyses described above have shown that ^{129}I is the dominant dose contributor for all the cases analyzed (two permeability cases and two waste inventory types). This is an expected outcome considering the key characteristics of ^{129}I relevant to geologic disposal of radioactive waste: unlimited solubility, no sorption or very weak sorption on typical geologic material, and extremely long half-life (about 17,000,000 yr). One approach to mitigate the potential release of ^{129}I is to load the seal materials with an effective sorbent for iodine. Careful studies would be needed to minimize passing any toxicity of the sorbent to near-surface groundwater.

Sensitivity analyses were conducted to evaluate potential impacts of iodine sorbent (getter) loaded in the seal zone on the deep borehole GDS performance. The sensitivity analyses were performed for the high permeability case because it yields the higher peak mean doses. The impact was analyzed with the linear sorption (Kd) model for iodine for a bentonite seal material. Uniform distribution with the bounds of 12 mL/g and 30 mL/g was used for the Kd for iodine in the seal zone, and the Kd value range is based on the best estimate from an on-going research (Krumhansl et al. 2011).

The analysis results for the commercial UNF inventory case are shown in Figures 3.4-25 to 3.4-27. Figure 3.4-25 shows the mean advective and diffusive mass release rates from the seal zone for the commercial UNF inventory case. The disposal zone mass releases are about the same as the case without iodine sorbent and are not shown because this zone is treated the same in both conceptualizations. As shown in Figure 3.4-25, the ^{129}I mean release rates from the seal zone are greatly suppressed while the mean release rates for other radionuclides remain about the same. The mean mass release rates from the upper zone (Figure 3.4-26) show that ^{129}I is no longer the dominant radionuclide, and ^{99}Tc and ^{36}Cl have higher mean mass release rates than ^{129}I. The peak mean dose at the hypothetical accessible environment is contributed mostly by ^{99}Tc and ^{36}Cl, no longer by ^{129}I (Figure 3.4-27). The total peak mean dose is reduced by about two orders of magnitude.

The analysis results for the DHLW inventory case are shown in Figures 3.4-28 and 3.4-29. Figure 3.4-28 shows the mean advective and diffusive mass release rates from the seal zone for the DHLW inventory case. The disposal zone mass releases are not shown as the releases are about the same as the case without iodine sorbent. The ^{129}I mean release rate is completely suppressed. ^{99}Tc is the only radionuclide that is released at a noticeable mean rate, and is the single dose contributor at the hypothetical accessible environment (Figure 3.4-29). The upper zone release results are not shown as they are about the same as those in the seal zone. The effect of ^{129}I suppression is demonstrated as the total peak mean dose is reduced by about six orders of magnitude. The performance benefit of an iodine sorbent in the seal zone is much greater for the DHLW case that for the commercial UNF inventory case under the high permeabilities associated with failed barriers.

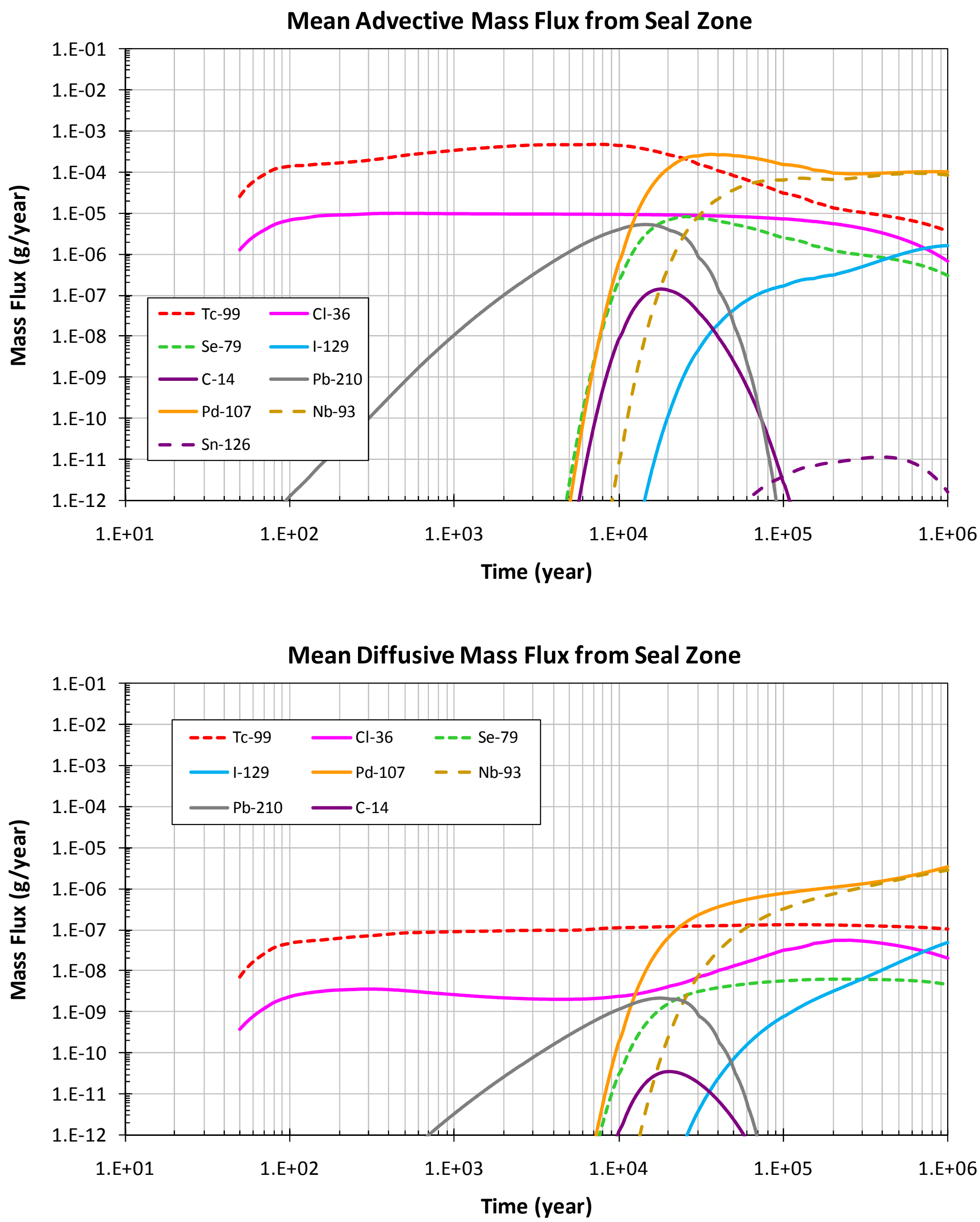


Figure 3.4-25. Commercial UNF Model Results for the High Permeability Case and Iodine Getter in Seal Zone: Mean Advective and Diffusive Mass Release Rate from Seal Zone

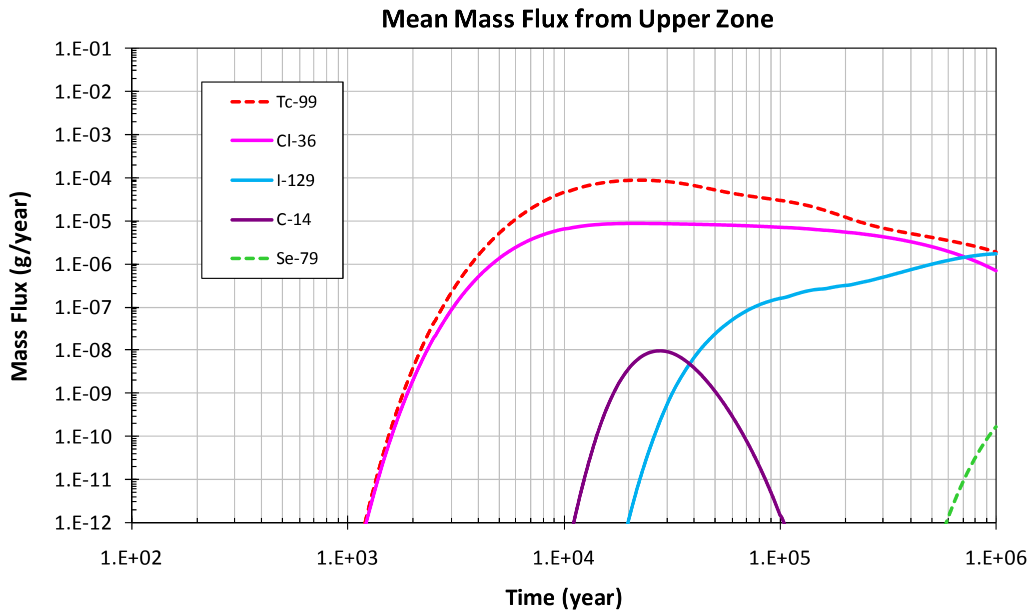


Figure 3.4-26. Commercial UNF Model Results for the High Permeability Case and Iodine Getter in Seal Zone: Mean Mass Release Rate from Upper Zone

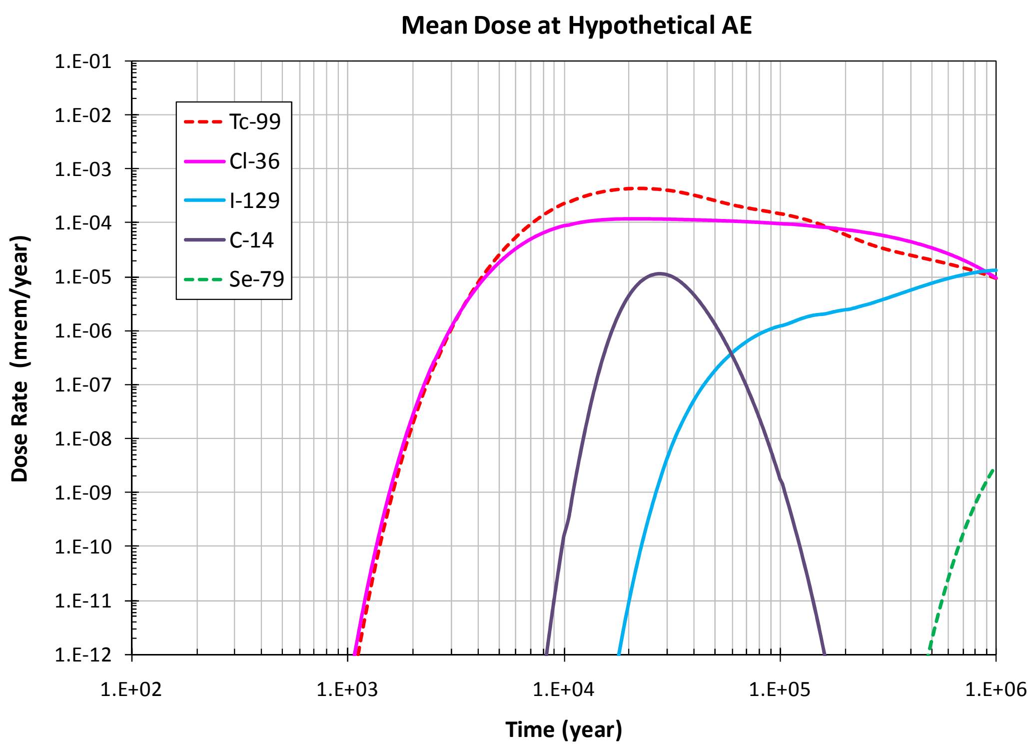


Figure 3.4-27. Commercial UNF Model Results for the High Permeability Case and Iodine Getter in Seal Zone: Mean Annual Dose at the Hypothetical Accessible Environment Located above the Repository

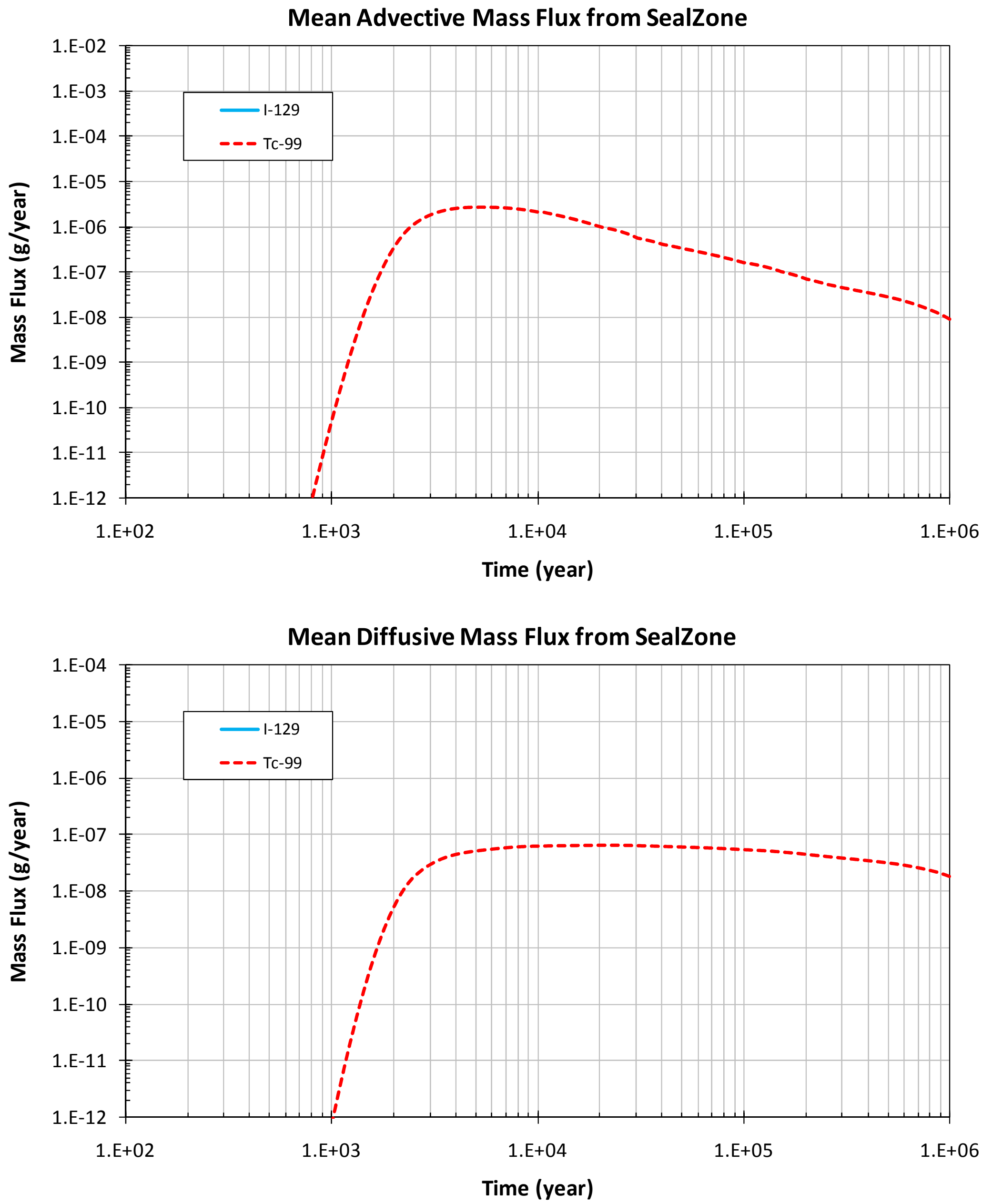


Figure 3.4-28. DHLW Model Results for the High Permeability Case and Iodine Getter in Seal Zone: Mean Advective and Diffusive Mass Release Rate from Seal Zone

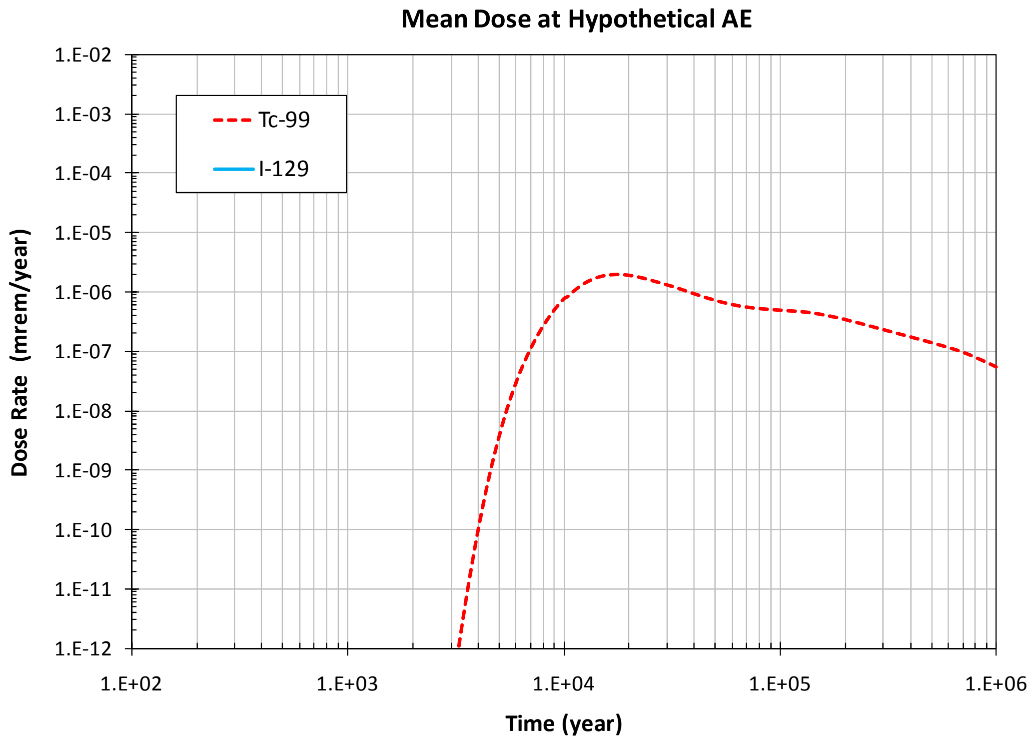


Figure 3.4-29. DHLW Model Results for the High Permeability Case and Iodine Getter in Seal Zone: Mean Annual Dose at the Hypothetical Accessible Environment Located above the Repository

3.4.3 Conclusions

A preliminary deep borehole GDS model has been developed to evaluate aspects of the long-term performance of deep borehole disposal concepts for UNF and HLW. The model is implemented in GoldSim software using the contaminant transport module. An external SNL 3D thermal hydrology process model is used to provide thermally driven, vertical groundwater fluxes. The current model does not include disruptive scenarios or borehole intrusion. Simplifications have also been made such as the assumption of immediate waste package failure, and in data usage. Results of the deep borehole GDS model were compared with an analytical solution for advective-dispersive transport as part of a confidence building exercise. The excellent agreement of the two methods shows that the deep borehole GDS model accurately simulates radionuclide transport in a deep borehole under the conditions tested. Preliminary simulations have also been made for three waste types and bounding permeability cases. These simulations were made to test the capability of the model. Future development of the modeling capability will include modeling of potential scenarios, use of more representative data, and inclusion of more representative process models. The capabilities of the deep borehole GDS model are being incorporated into the GPAM (Section 4) along with the capabilities of models for the salt, granite, and clay repository options. Future changes to modeling of these options will be made directly in the GPAM. When completed, GPAM can be used to provide decision makers with risk information to defensible support viability studies, option screening, prioritization of research needs, and other programmatic strategies.

4. GPAM ARCHITECTURE DEVELOPMENT

Preliminary development of GPAM was initiated in FY 2011. The objective of the GPAM is to create a single model framework that is common to the range of disposal system alternatives that might potentially be considered within the UFD Campaign and that can accommodate scientific representations of relevant phenomena at varying levels of detail or complexity dependent on end use. Freeze et al. (2010, Section 2.1) identified 35 potential UFD disposal and storage system alternatives based on combinations of five potential (current and future) waste form types and seven potential design concepts/geologic settings. The initial focus of GDSM is on four UNF and HLW waste form types (Table 4-1) and on the five mined and deep disposal concepts (Table 4-2), for a total of 20 UFD disposal system alternatives[b].

Table 4-1. Potential Waste Form Types Considered in GPAM

Waste Form Type	Description
Used Nuclear Fuel (UNF)	e.g., Commercial, DOE-owned, high temperature gas reactor
High-Level Waste (HLW) Glass	Current (e.g., borosilicate) and future (e.g., no minor actinides)
High-Level Waste (HLW) Glass Ceramic / Ceramic	Current (glass-bonded sodalite) and future (e.g., from electrochemical processing)
High-Level Waste (HLW) Metal Alloy	From electrochemical or aqueous reprocessing, cermets

Table 4-2. Potential Disposal Concepts and Geologic Settings Considered in GPAM

Disposal Concept / Geologic Setting	Description
Mined Geologic Disposal (Hard Rock, Unsaturated)	Granite/crystalline or tuff (depths > 100 m)
Mined Geologic Disposal (Hard Rock, Saturated)	Granite/crystalline or tuff (depths > 100 m)
Mined Geologic Disposal (Clay/Shale, Saturated)	Clay/shale (depths > 100 m)
Mined Geologic Disposal (Salt, Saturated)	Bedded or domal salt (depths > 100 m)
Deep Borehole Disposal	Granite/crystalline (depths ~1000 m or deeper)

In FY 2010, these 20 UFD disposal system alternatives were represented by four individual GDS models (Wang and Lee 2010): granite, clay, salt, and deep borehole. The focus of the four individual GDS models was on the disposal concept and geologic setting and, therefore, the options to examine different waste form types were limited, although a common source term and biosphere was used in some of the models (Wang and Lee 2010; Chapter 1). Continuing FY 2011 development of these four individual GDS models is described in Section 3. Future development and implementation of these individual GDS models will occur within the GPAM framework. Note that the discussions in Section 3 tend to emphasize the waste form/stream options (commercial UNF, DHLW, and CHLW) rather than the corresponding

[b] The preliminary version of GPAM assumes a fluid saturation of 1in all model domains. The capability for unsaturated domains will be added in a future version.

waste form types shown in Table 4-1. For commercial UNF, there is no difference. However, for DHLW and CHLW, the corresponding waste form type is assumed to be HLW glass, specifically borosilicate glass.

The GPAM was developed to provide a tool to efficiently combine any of the four waste form types and any of the five disposal concepts and geologic settings within a single conceptual framework. The single, common GPAM conceptual framework enables evaluations and comparisons of disposal system alternatives to be made with as many common system components as needed. Representations of the system components and associated phenomena can range from simple abstractions to complex coupled processes. The GPAM framework also facilitates the use of a common parameter database for input values (Section 4.2.2.2) and a common configuration management system (Section 4.2.3) to provide consistency in comparisons and a controlled computational environment.

4.1 GPAM Concept

The GPAM conceptual framework is organized around four common disposal system regions (Figure 4-1): Source; Near Field; Far Field; and Biosphere. Each of the four GPAM Regions, in turn, consists of one or more common features. Figure 4-1 also illustrates the relationship between the GPAM Regions and alternate terms that are commonly used to describe a disposal system: EBS, geosphere, and biosphere. The near field encompasses the EBS and as well as the interface with, and adjacent portion of, the host rock that experiences durable (but not necessarily permanent) changes due to the presence of the repository (e.g., hydro-mechanical alteration due to excavation, thermal-chemical alteration due to waste emplacement). The far field encompasses the remainder of the geosphere. The receptor is located within, and has behaviors and characteristics consistent with, the biosphere.

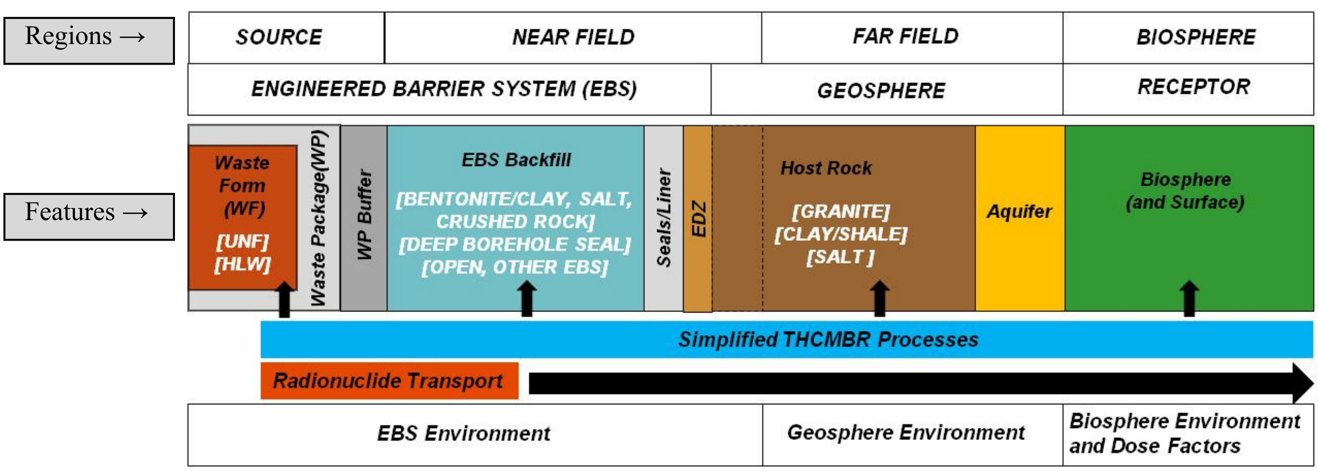


Figure 4-1. Schematic Illustration of GPAM Regions, Features, and Phenomena

The bottom half of Figure 4-1 illustrates how radionuclide movement from the waste form to the biosphere is influenced by phenomena that can act upon and within each of the GPAM Regions and Features. These phenomena include, at a high level, the THCMBR processes and external events (e.g., seismicity) that describe (1) waste degradation and radionuclide release from the Source Region, (2) radionuclide transport through the Near-Field and Far-Field Regions, and (3) radionuclide transport, uptake, and health effects in the Biosphere Region. In addition to their direct effects on radionuclide transport, the THCMBR processes also influence the physical and chemical environments (e.g., temperature, fluid chemistry, biology, mechanical alteration) in the EBS, geosphere, and biosphere, which in turn affect water movement, degradation of EBS components, and radionuclide transport.

These generic GPAM Regions and Features, and the associated THCMBR processes and events, are consistent with the generic features defined in the UFD FEP list (Freeze et al. 2010). As described in Freeze et al. (2010, Section 2), the UFD FEP list derived from a Nuclear Energy Agency (NEA) FEP list (NEA 1999; 2006) that included phenomena from 10 different national radioactive waste disposal programs covering a wide range of waste forms, disposal concepts, and geologic settings. As a result, the UFD FEP list represents a wide range of disposal system alternatives. Correspondingly, the generic GPAM Regions and Features are a comprehensive set spanning a wide range of potential disposal options and can be used to represent any of the 20 UFD disposal system alternatives. This flexibility is supported by the FEP mapping in Section 2.

General characteristics of each of the four GPAM Regions are described below:

- *Source Region*—Contains the waste inventory, waste form, waste package, and waste package buffer features. The radionuclide source term derives from the waste form and waste package degradation mechanisms, which are a function of the EBS environment (temperature, fluid chemistry, and physical conditions). The Source Region provides a radionuclide flux to the Near Field Region.
- *Near-Field Region*—Contains some or all of the following features: engineered backfill, open tunnels, seals, liner, EDZ, and near-field host rock. Radionuclide transport through the Near Field Region is a function of the EBS environment, fluid flow, and flow path properties. The Near Field Region provides a radionuclide flux to the Far Field Region. Fluid flow to the Source Region may also occur through the Near Field Region.
- *Far-Field Region*—Contains the far-field host rock and surrounding geologic units (represented by an aquifer). Radionuclide transport through the Far-Field Region is a function of geosphere environment, fluid flow, and flow path properties. The Far-Field Region provides a radionuclide flux to the Biosphere Region. Fluid flow to the Near-Field Region may also occur through the Far-Field Region.
- *Biosphere Region*—Contains the individual(s) and/or community and the associated surface conditions representative of a human receptor. Radionuclide flux to the Biosphere Region is used to determine associated human health effects. Human health effects are quantified in terms of an annual radionuclide dose to the receptor.

To perform quantitative disposal system evaluations, mathematical models of the GPAM conceptual framework and the associated FEPs are needed. At this early stage of the UFD Campaign, simple mathematical representations of the FEPs (e.g., reduced-dimension geometry, minimal THCMBR process coupling) are sufficient to demonstrate modeling capabilities, perform scoping studies, and provide high-level evaluations of GDS alternatives. The simple GPAM representation also supports inclusion into high-level system evaluations of fuel cycle options (Sevougian et al. 2011). As the UFD Campaign matures, more complex mathematical representations of the FEPs (3D, robust process coupling) will likely be needed to provide more detailed analyses of specific disposal system sites and/or design components. These representations and the data needed to support them will come from other UFD work packages (e.g., EBS, Natural Systems). Associated with more complex mathematical representations is the potential application of high-performance computing (HPC) methods. Preliminary efforts to develop HPC-based complex mathematical representations applicable to disposal system modeling are documented in Freeze et al. (2011b) (focused on the EBS) and DOE (2010a) (focused on the geosphere).

The preliminary GPAM employs simple mathematical representations of the generic FEPs as described in Section 4.1.1. However, the GPAM conceptual framework is modular in the sense that complexity can be introduced progressively, Region by Region. Therefore, more complex representations of specific disposal system features, components, and/or entire Regions can be introduced as is necessary (e.g., to further investigate specific high-level FEPs shown to be important in simple generic representations.

4.1.1 Simple Mathematical Representations

The preliminary GPAM employs simple mathematical representations of waste degradation and radionuclide release from the Source Region (Section 4.1.1.1), radionuclide transport through the Near-Field and Far-Field Regions (Section 4.1.1.2), and radionuclide uptake and health effects in the Biosphere Region (Section 4.1.1.3). As noted in Section 4.1, these simple mathematical representations provide an initial technical basis for the GPAM. More complex representations can be implemented as needed.

4.1.1.1 Radionuclide Source Term

The simple mathematical representation of the radionuclide source term considers an initial radionuclide inventory, radionuclide decay and ingrowth, waste package failure times (for initiation of waste form degradation), fractional waste form degradation rates (for waste degradation and dissolution) and radionuclide solubility limits (for radionuclide mobilization). The combination of these processes produces temporal and spatial distributions of radionuclide masses in the Source Region (1) dissolved in the water in the void volume (i.e., the radionuclide source concentration) and (2) in various solid forms (e.g., undegraded waste, precipitated, sorbed).

In this simple mathematical representation, the radionuclide source term provides input to the radionuclide transport calculations in the Near Field region (Section 4.1.1.2). In addition, some of the factors controlling the source term (e.g., water availability, degradation rates, solubility limits) are dependent on the characteristics of the Near-Field and Far-Field Regions. However, in this simple representation there is no explicit, dynamic coupling between the Source Region and Near Field Region.

4.1.1.2 Radionuclide Transport

The simplified mathematical representation of radionuclide transport considers advection, hydrodynamic dispersion (molecular diffusion and mechanical dispersion), sorption, and decay. The combination of these processes produces temporal and spatial distributions of radionuclide masses in the Near Field and Far-Field Regions (1) dissolved in the water in the pore volume (i.e., the dissolved radionuclide concentration) and (2) in various solid forms (e.g., precipitated, sorbed).

Radionuclide transport through porous media can be represented by the advection-dispersion equation, which describes the mass balance between the advective mass flux through, the dispersive mass flux through, and the rate of mass change within a volume of porous medium. The 1D form of the mass balance for nonreactive dissolved radionuclides in a saturated, homogeneous, isotropic medium under steady-state, uniform flow is (Freeze and Cherry 1979, Equation A10.7; Domenico and Schwartz 1990, Equation 13.7; Schwartz and Zhang 2003, Equation 23.10; de Marsily 1986, Equation 10.1.5):

$$\frac{\partial (Cn)}{\partial t} = \frac{\partial}{\partial x}\left(nD_x \frac{\partial C}{\partial x} \right) - \frac{\partial (nv_x C)}{\partial x} \quad \text{Eq. 4-1}$$

where:

C = dissolved radionuclide concentration [M/L^3]

x = distance in direction of groundwater flow [L]

t = time [T]

n = porosity [ ]

v_x = groundwater pore velocity [L/T]

D_x = coefficient of hydrodynamic dispersion [L^2/T]

In Equation 4-1, the left-hand side represents the rate of mass change (gain) [M/L3·T] (Freeze and Cherry 1979, p. 551; Domenico and Schwartz 1990, Equation 13.1; Schwartz and Zhang 2003, Equation 23.7), the second right-hand-side term represents the mass flux (loss) due to advection [M/L3·T] (Freeze and Cherry 1979, Equation A10.1; Domenico and Schwartz 1990, Equation 10.1; Schwartz and Zhang 2003, Equation 19.2), and the first right-hand-side term represents the mass flux (gain) due to hydrodynamic dispersion [M/L3·T] (Freeze and Cherry 1979, Equation A10.2; Domenico and Schwartz 1990, Equation 10.11; Schwartz and Zhang 2003, Equation 19.9).

In a homogeneous medium that does not change over time, the mass balance in Equation 4-1 simplifies to the 1D form of the advection-dispersion equation for nonreactive dissolved radionuclides (Freeze and Cherry 1979, Equation 9.3; Domenico and Schwartz 1990, Equations 13.13 and 17.1; Schwartz and Zhang 2003, Equation 23.10; de Marsily 1986, Equation 10.1.6):

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} \qquad \text{Eq. 4-2}$$

The advection term in Equations 4-1 and 4-2 captures the effects of transport by flowing groundwater, by assuming that the nonreactive (i.e., nonsorbing) radionuclide center of mass moves at the groundwater pore velocity, v_x. The groundwater pore velocity (also referred to as linear groundwater velocity), derives from the Darcy velocity (also referred to as specific discharge), v_D [L/T] (Freeze and Cherry 1979, p. 389):

$$v_x = \frac{v_D}{n} \qquad \text{Eq. 4-3}$$

The Darcy velocity derives from Darcy's Law (Freeze and Cherry 1979, p. 16):

$$v_D = Ki \qquad \text{Eq. 4-4}$$

and (Freeze and Cherry 1979, p. 27):

$$K = \frac{k\rho g}{\mu} \qquad \text{Eq. 4-5}$$

where:

K = hydraulic conductivity [L/T]

i = hydraulic gradient [ ]

k = permeability [L^2]

ρ = fluid density [M/L^3]

g = gravitational constant [L/T^2]

μ = fluid viscosity [M/L·T]

The hydrodynamic dispersion term in Equations 4-1 and 4-2 captures the effects of radionuclide spreading around the center of mass. Hydrodynamic dispersion combines the effects of mixing due to mechanical dispersion and of molecular diffusion in response to a concentration gradient (Freeze and Cherry 1979, Equation 9.4; Domenico and Schwartz 1990, Equations 10.8 and 10.17; Schwartz and Zhang 2003, Equation 23.18; de Marsily 1986, p. 239):

$$D_x = \alpha_x v_x + D_b \qquad \text{Eq. 4-6}$$

where:

α_x = longitudinal dispersivity [L]

D_b = bulk diffusion coefficient (for a radionuclide in a porous medium) [L^2/T]

The first term in Equation 4-6 represents mixing due to mechanical dispersion. In Equation 4-2 these effects of dispersive mixing are defined as a function of a concentration gradient (i.e., in terms of Fick's Law). Therefore, this mathematical formulation of mechanical dispersion is often referred to as Fickian dispersion. The selection of representative values for longitudinal dispersivity is generally thought to be scale-dependent (Freeze and Cherry 1979, pp. 400-01, 430-31; Domenico and Schwartz 1990, pp. 369-77; Schwartz and Zhang 2003, pp. 450-58; de Marsily 1986, pp. 247-51). A reasonable rule of thumb is that, for transport distances up to about 1000 m, the longitudinal dispersivity is about one-tenth of the transport distance (Schwartz and Zhang 2003, Figure 19.10).

The second term in Equation 4-6 represents the diffusion of a radionuclide in the porous medium. The diffusion of a radionuclide in a nonreactive (i.e., nonsorbing) porous medium, represented by the bulk diffusion coefficient, D_b, is related to, but smaller than, the diffusion of a radionuclide in a pure fluid, represented by the free water diffusion coefficient, D_w [L^2/T]. Values for the free water diffusion coefficient range from about 5×10^{-10} m^2/s to 2×10^{-9} m^2/s for major ions at 25°C (Schwartz and Zhang 2003, Table 19.1), with values about 50% lower at 5°C (Freeze and Cherry 1979, p. 103). Diffusion in a porous medium is less than in a pure fluid because the solid medium stops the Brownian movement of the diffusing particles (de Marsily 1986, p. 233) and there are correspondingly longer diffusion paths through porous media (Freeze and Cherry 1979, p. 103). The reduction in diffusion is greater in denser media (e.g., clay) that have more tortuous diffusion paths, than in looser media (e.g., sand). The relationship between the bulk diffusion coefficient and the free water diffusion coefficient is typically quantified by (Domenico and Schwartz 1990 Equation 10.16; Schwartz and Zhang 2003, Equation 19.8; de Marsily 1986, p. 233):

$$D_b = \tau \, D_w \qquad \text{Eq. 4-7}$$

where:

τ = tortuosity [ ]

The tortuosity, τ, represents the reduction fraction and is defined as the ratio of porous medium length to flow channel length (Domenico and Schwartz 1990, p. 368; Bear 1972, p. 110)[c]. Therefore, the value of τ is always less than one, and as the flow channel lengths (i.e., diffusion paths) become more tortuous, the value of τ gets smaller. Despite the formal definition presented above, tortuosity is difficult to quantify and in practice is somewhat of an empirical coefficient. The tortuosity in a saturated medium is often assumed to be a function of the porosity (Schwartz and Zhang 2003, Equation 19.7):

$$\tau = n^{1/3} \qquad \text{Eq. 4-8}$$

[c] In some literature, tortuosity is defined inversely (i.e., as the ratio of flow channel length to porous medium length) or in relation to constrictivity, δ. See, for example, Equation A-3.

The relationship in Equation 4-8 results in values of τ ranging from about 0.7 (for a porosity of 0.35) to 0.2 (for a porosity of 0.01). For comparison, observations of the reduction fraction in porous media range from 0.8 to 0.01 (Freeze and Cherry 1979, p. 104; Domenico and Schwartz 1990, p. 368; Schwartz and Zhang 2003, p. 447; de Marsily 1986, p. 233; Bear 1972, p. 111), with fractions most commonly ranging from about 0.7 to 0.1. It should be noted that an additional reduction in diffusion through a porous medium, beyond the effects of tortuosity, is caused by sorption of radionuclides onto the solids (Freeze and Cherry 1979, p. 103-04). This effect is discussed later as part of the apparent diffusion coefficient (Equation 4-25).

Diffusion is sometimes reported in terms of an effective diffusion coefficient, D_e [L^2/T], where:

$$D_e = nD_b = n\tau \; D_w \qquad \text{Eq. 4-9}$$

The form of the effective diffusion coefficient is consistent with the form of dispersive mass flux (first right-hand-side term in Equation 4-1). Because laboratory diffusion experiments often measure diffusive mass flux, their results are often effective diffusion coefficients rather than bulk diffusion coefficients. In these cases, the laboratory effective diffusion coefficients need to be adjusted by a factor of the porosity, n, for use in the advection-dispersion equation (Equations 4-2 and 4-6).

The effective diffusion coefficients defined in Equations 3.3-1, 3.3-2, 3.3-6, 3.3-7, 3.3-11, 3.3-13, and 3.3-15 and used in the clay GDS model are consistent with Equation 4-9.

The form of Equation 4-6 indicates the relative contributions of advection (v_x), mechanical dispersion (α_x), and diffusion (D_b) to transport. A dimensionless Peclet number, N_{PE}, is sometimes used to quantify these relationships, where (Freeze and Cherry 1979, p. 392; Domenico and Schwartz 1990, p. 371; de Marsily 1986, p. 237):

$$N_{PE} = \frac{v_x d}{D_b} \qquad \text{Eq. 4-10}$$

where:

d = characteristic length of porous media (e.g., particle or pore diameter) [L]

A low Peclet number indicates diffusion-dominated transport (and that hydrodynamic dispersion is dominated by diffusion), whereas a high Peclet number indicates advection-dominated transport (and that hydrodynamic dispersion is dominated by mechanical dispersion).

A reaction term, r [$M/L^3 \cdot T$], can be added to Equation 4-1 to account for the effects (i.e., losses from the dissolved mass) of sorption and decay in the 1D advection-dispersion mass balance for radionuclides in a saturated, homogeneous, isotropic medium under steady-state, uniform flow (Schwartz and Zhang 2003, Equation 23.11; de Marsily 1986, Equation 10.2.1):

$$\frac{\partial (Cn)}{\partial t} = \frac{\partial}{\partial x}\left(nD_x \frac{\partial C}{\partial x} \right) - \frac{\partial (nv_x C)}{\partial x} - r \qquad \text{Eq. 4-11}$$

The effects of sorption of radionuclides onto the porous medium are represented with the reaction term in Equation 4-11 by (Freeze and Cherry 1979, Equation 9.9; Domenico and Schwartz 1990, Equations 13.17 and 13.21; Schwartz and Zhang 2003, Equation 23.12; de Marsily 1986, pp. 252-60):

$$r = \rho_b \frac{\partial S}{\partial t}$$ Eq. 4-12

where:

ρ_b = bulk density of porous medium [M/L^3]

S = mass of radionuclide sorbed per unit mass of porous medium [ ]

Equation 4-12 is sometimes written in terms of the solid density of the porous medium, ρ_s [M/L^3], where:

$$\rho_b = (1 - n)\rho_s$$ Eq. 4-13

The simple mathematical representation assumes that the relationship between the sorbed radionuclide mass and the dissolved radionuclide mass is represented by a linear isotherm (Freeze and Cherry 1979, Equation 9.12; Domenico and Schwartz 1990, Equation 13.23; de Marsily 1986, p. 256):

$$S = k_d C$$ Eq. 4-14

where:

k_d = distribution coefficient [L^3/M]

The distribution coefficient, k_d, quantifies the partitioning of radionuclides between the sorbed phase and the dissolved phase. A larger k_d indicates that a larger proportion of the radionuclide mass is sorbed.

Combining Equations 4-12 and 4-14 gives:

$$r = \rho_b k_d \frac{\partial C}{\partial t}$$ Eq. 4-15

The effects of sorption of radionuclides onto the porous medium can also be quantified in terms of a retardation factor, R_f (Freeze and Cherry 1979, Equation 9.14; Domenico and Schwartz 1990, Equations 13.26; Schwartz and Zhang 2003, Equation 23.14; de Marsily 1986, Equation 10.2.3):

$$R_f = 1 + \frac{\rho_b k_d}{n}$$ Eq. 4-16

Care should be taken when interpreting reported values of retardation factors and distribution coefficients from laboratory or field tests. Distribution coefficients tend to lump together multiple equilibrium and kinetic reactions (i.e., not limited to sorption) and are specific to the conditions under which they were measured (e.g., pH, ionic strength, temperature, fluid-to-rock ratio, medium type, etc.). Measured distribution coefficients therefore provide only a rough predictor of the potential for radionuclide retardation (McKinley and Scholtis 1993; Bethke and Brady 2000).

The effects of first-order decay of the dissolved radionuclide mass are represented with the reaction term in Equation 4-11 by (Domenico and Schwartz 1990, Equation 13.15; de Marsily 1986, Equation 10.3.2):

$$r = \lambda(Cn) \quad \text{Eq. 4-17}$$

where:

λ = radioactive decay constant [T^{-1}]

In addition, when considering the combined effects of sorption and radionuclide decay, the effects of first-order decay of the sorbed radionuclide mass are represented by (de Marsily 1986, Equation 10.2.7):

$$r = \lambda(\rho_b S) \quad \text{Eq. 4-18}$$

Substituting Equation 4-14 into Equation 4-18 yields:

$$r = \lambda(\rho_b k_d C) \quad \text{Eq. 4-19}$$

Substituting Equation 4-15, Equation 4-17, and Equation 4-19 into Equation 4-11 yields:

$$\frac{\partial(Cn)}{\partial t} + \rho_b k_d \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(nD_x \frac{\partial C}{\partial x}\right) - \frac{\partial(nv_x C)}{\partial x} - \lambda Cn - \lambda \rho_b k_d C \quad \text{Eq. 4-20}$$

Combining like terms and substituting Equation 4-16 into Equation 4-20 yields the final 1D form of the mass balance for reactive (i.e., sorbing and decaying) radionuclides in a saturated, homogeneous, isotropic medium under steady-state, uniform flow (Schwartz and Zhang 2003, Equation 23.15; de Marsily 1986, Equation 10.2.8):

$$nR_f \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(nD_x \frac{\partial C}{\partial x}\right) - \frac{\partial(nv_x C)}{\partial x} - nR_f \lambda C \quad \text{Eq. 4-21}$$

The corresponding 1D form of the advection-dispersion equation for reactive radionuclides, which includes the effects of advection, dispersion, diffusion, sorption, and radionuclide decay, is (Schwartz and Zhang 2003, Equation 23.27; de Marsily 1986, Equation 10.3.3):

$$R_f \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} - R_f \lambda C \quad \text{Eq. 4-22}$$

For comparison with the nonreactive form of the advection-dispersion equation (Equation 4-2), Equation 4-22 can be written as:

$$\frac{\partial C}{\partial t} = \left(\frac{D_x}{R_f}\right)\frac{\partial^2 C}{\partial x^2} - \left(\frac{v_x}{R_f}\right)\frac{\partial C}{\partial x} - \lambda C \quad \text{Eq. 4-23}$$

The form of Equation 4-23 leads to the definition of two additional properties: apparent velocity, v_a [m/yr], and apparent diffusion coefficient, D_a [L^2/T]. The apparent velocity represents the effective velocity of a sorbing radionuclide through the porous medium:

$$v_a = \frac{v_x}{R_f} \qquad \text{Eq. 4-24}$$

The apparent velocity is not a physical velocity, rather it represents the combined effects of a radionuclide alternately flowing through the pore space at the groundwater pore velocity and being delayed due to sorption onto and subsequent desorption from the porous medium.

The apparent diffusion coefficient captures the additional reduction in diffusion through a porous medium that is caused by sorption of radionuclides onto the solids (Freeze and Cherry 1979, p. 103-04)[d]:

$$D_a = \frac{D_b}{R_f} = \frac{\tau \ D_w}{R_f} \qquad \text{Eq. 4-25}$$

Combining Equation 4-24 and Equation 4-25 with Equation 4-6 yields:

$$\frac{D_x}{R_f} = \alpha_x v_a + D_a = \alpha_x v_a + \frac{\tau \ D_w}{R_f} \qquad \text{Eq. 4-26}$$

As with retardation factors and distribution coefficients, care should also be taken when interpreting reported values of diffusion coefficients from laboratory or field tests. Measured values for diffusion coefficients in porous media tend to lump together the effects of the solid medium (e.g., tortuous diffusion paths, collisions with solids) and thermo-chemical effects (e.g., sorption and other reactions) and are also specific to the conditions and medium type. Also, the full effects of retardation may not always be captured in the measurements. Measured diffusion coefficients in porous media are most commonly representative of apparent diffusion coefficients (Equation 4-25). However, diffusion experiments often measure diffusive mass flux and the corresponding experimentally-derived diffusion coefficients need to be adjusted by a factor of the porosity, *n*, for use in the advection-dispersion equation (Equation 4-23 and Equation 4-26).

The numerical solution of Equation 4-23 produces temporal and spatial distributions of dissolved radionuclide concentrations in the Near-Field and Far-Field Regions and radionuclide mass fluxes between regions. Sorbed radionuclide masses are calculated from Equation 4-14. Precipitated radionuclide masses are dependent on the radionuclide solubilities.

In this simple mathematical representation, the radionuclide mass fluxes provide input to the radionuclide dose calculations in the Biosphere Region (Section 4.1.1.3). However, in this simple representation there is no explicit, dynamic coupling between the Far-Field Region and Biosphere Region.

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[d] In some literature, the apparent diffusion coefficient is defined as $D_a = D_e / R_f = n\tau D_w / R_f$. This alternate definition differs from Equation 4-25 by a factor of the porosity, *n*.

4.1.1.3 Radionuclide Dose

The simplified mathematical representation of radionuclide dose considers dilution rate, water consumption rate, and dose coefficients. The combination of these parameters produces time-dependent annual radionuclide doses in the Biosphere Region.

The GPAM dose calculation is based on the IAEA BIOMASS ERB 1B dose model (IAEA 2003, Sections A.3.2 and C.2.6.1). The ERB 1B dose model assumes that the receptor is an individual adult who obtains his drinking water from a pumping well drilled into the Far-Field Region. The dissolved radionuclide concentration in water withdrawn from the pumping well, C_W [M/L^3] is:

$$C_W = \frac{Q_{FF}}{q_D} \qquad \text{Eq. 4-27}$$

where:

Q_{FF} = radionuclide mass flux from the Far-Field Region [M/T]

q_D = volumetric dilution/pumping rate [L^3/T]

The annual dose to the receptor from a specific radionuclide, H_R [Sv/yr], is (IAEA 3002, p. 300):

$$H_R = (C_W a)(I)(dcf) \qquad \text{Eq. 4-28}$$

where:

I = annual volumetric consumption rate of drinking water from well by receptor [L^3/yr]

dcf = ERB1 radionuclide-specific dose coefficient [Sv/Bq]

a = radionuclide-specific activity [Bq/M]

Equations 4-27 and 4-28 are sometimes formulated in terms of radionuclide-specific dose conversion factor, DCF [(Sv/yr)/(Bq/yr)]:

$$DCF = (dcf)\left(\frac{I}{q_D}\right) \qquad \text{Eq. 4-29}$$

When written in terms of DCF, the annual dose to the receptor, H_R, from Equation 4-28 is the following:

$$H_R = (Q_{FF} a)(DCF) \qquad \text{Eq. 4-30}$$

4.2 GPAM Implementation

The GPAM conceptual framework for a GDS described in Section 4.1 was implemented in GoldSim (GoldSim Technology Group 2010c). The GoldSim Contaminant Transport Module (GoldSim Technology Group 2010a) provides numerical solutions to the simple mathematical representations identified in Section 4.1.1. The preliminary GoldSim implementation, referred to as GPAM Version 0 (V0), requires the specification of the following model components:

- *Input File*—Input parameter deterministic values and/or probability distributions are maintained and selected using an external file. For GPAM V0, the external file is an MS Excel spreadsheet. Each simulation requires the same set of input parameters, but the specific values differ based on the disposal alternative they represent. Details of the MS Excel input file are described in Section 4.2.2.1. An external parameter database is currently under development (Section 4.2.2.2) for implementation in future versions of the GPAM.
- *GoldSim Model File*—Implementation of the GPAM conceptual framework in GoldSim uses various GoldSim transport elements (e.g., Cells and Pipes) to represent the THCMBR phenomena that govern fluid flow and radionuclide transport through the GPAM Regions (i.e., to provide numerical solutions to the equations in Section 4.1.1). Details of the GPAM Regions and subregions (called GPAM domains) that include these transport elements are described in Section 4.2.1. Each of the four individual GDS models described in Section 3 can be implemented in GPAM by mapping to the individual model components to the generic GPAM Regions and Model Domains (see Section 4.3).
- *GoldSim Simulation Settings*—GoldSim simulation settings (e.g., time stepping, solution precision) are specified within GoldSim in GPAM V0. Details of the specification of simulation settings are described as part of the system-level input specifications in Section 4.2.2.
- *GoldSim Results Files*—Model results for the entire system (e.g., dose) as well as mass balances and fluxes within and between GPAM domains will be captured in GoldSim result elements and stored in results files. Details of the results files are described in Section 4.2.11.

These GPAM components are all accessed using the GoldSim Dashboard capability, from the home "page" of GPAM V0 GoldSim File. The home "page", referred to as the GPAM Main Dashboard, is shown in Figure 4-2.

4.2.1 GPAM GoldSim Model File

The GPAM GoldSim model file (Generic_PA_Model_R00.gsm) represents a single transport pathway through a disposal system with a series of GoldSim transport elements (e.g., Cells and Pipes). To provide the flexibility to represent different disposal concepts containing various combinations of features, the GoldSim transport elements are grouped into a generic set of eight GPAM domains. The spatial relationship between these eight GPAM domains and the GPAM regions and features is shown in Figure 4-3.

Each GPAM domain is characterized by one or more GoldSim transport elements (cells and/or pipes) and a set of parameters that describe its geometry, solid properties, fluid properties, transport properties, and, if needed, fracture properties. GoldSim cells and pipes provide a numerical solution to the advection-dispersion equation for reactive radionuclides (Equation 4-23). The numerical solution for pipes (GoldSim Technology Group 2010a, Appendix B, pp. 299-322) better represents advective-dominated transport (e.g., through fractured granite), whereas the numerical solution for cells (GoldSim Technology Group 2010a, Appendix B, pp. 282-299) better represents diffusive-dominated transport (e.g., through bentonite or clay). Through the selection of appropriate GoldSim transport elements and parameter values, a GPAM region can be conceptualized to represent most engineered materials and/or geologic

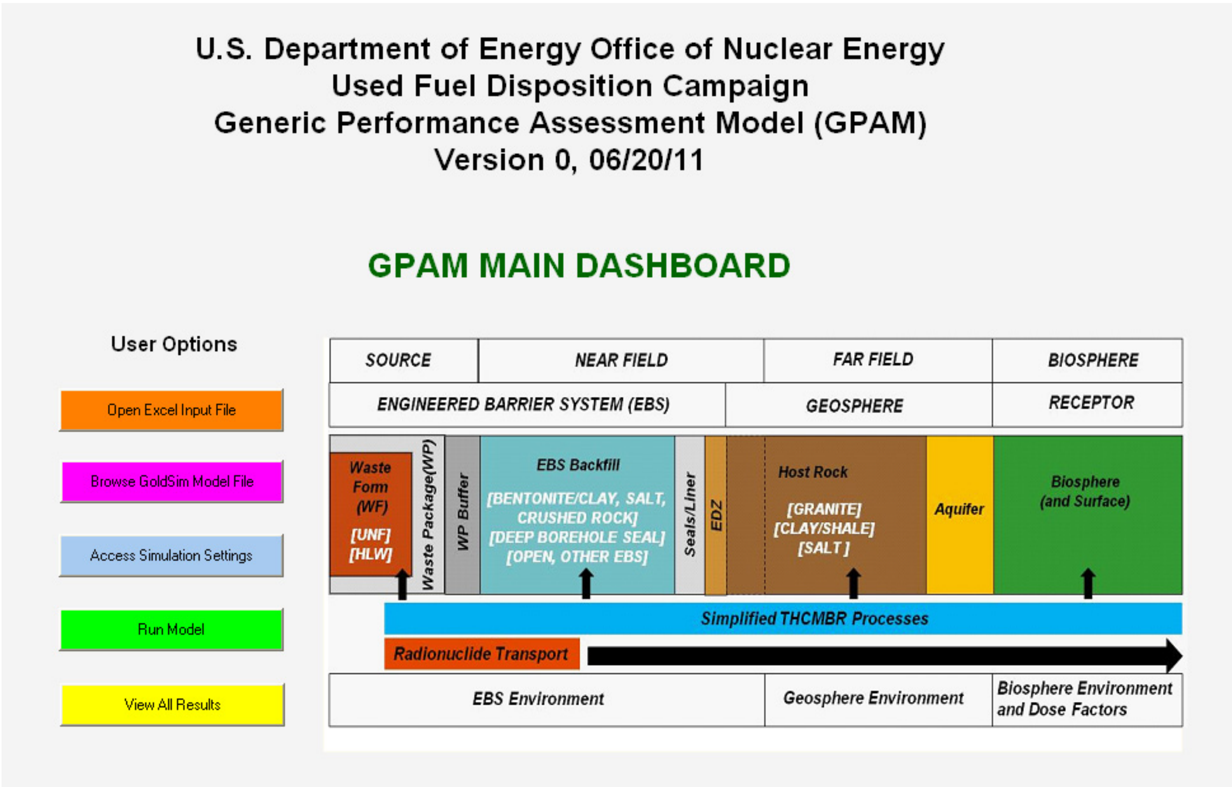


Figure 4-2. GoldSim GPAM Main Dashboard

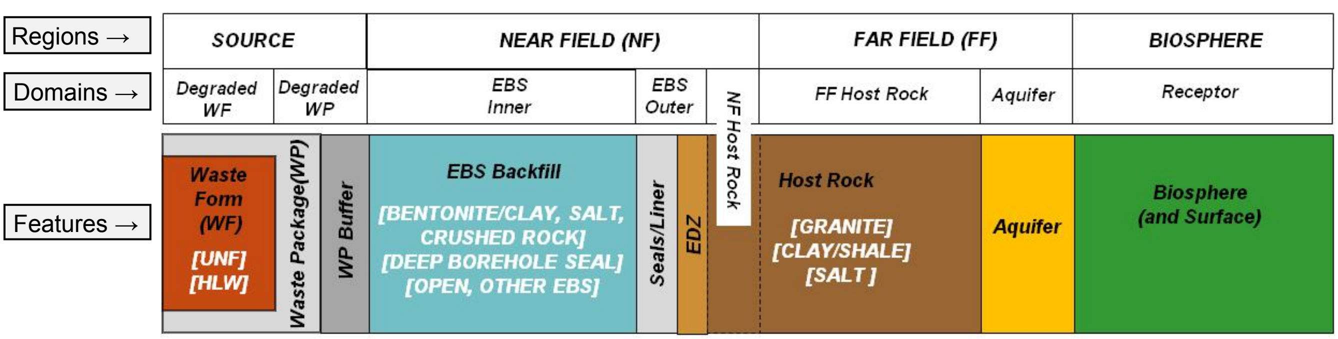


Figure 4-3. GoldSim GPAM Domains, Regions, and Features

media. Details of the specific transport elements and capabilities in each of the eight GPAM domains are described in Sections 4.2.1.2 through 4.2.1.9. Details of specific input parameters are described in Section 4.2.2.

In addition to the eight GPAM domains, a set of system-level specifications is required to fully characterize a disposal system. System-level specifications include radionuclide species and properties, reference fluid properties, system configuration, as well as libraries of properties that may be used in the characterization of the eight model domains (e.g., inventory, solubility, sorption, diffusivity, and dose factors). Details of the system-level specifications are described in Sections 4.2.1.1. The GPAM also provides the capability to simulate a fast pathway that may bypass one or more of model domains. Details of the specific transport elements and capabilities of the fast pathway are described in Section 4.2.1.10.

A summary of the system-level specifications, the GoldSim transport elements and capabilities of the eight GPAM domains, and the GoldSim transport elements and capabilities of the fast pathway is presented in Table 4-3.

The GoldSim representation of the GPAM model file is shown in Figure 4-4. The GoldSim model file is accessed from the GPAM Main Dashboard (Figure 4-2), and also provides a hyperlink back to the Main Dashboard. Within the GoldSim model file, there are containers corresponding to the input parameters (Section 4.2.2), the Source Region (Figure 4-5 and Sections 4.2.1.2 and 4.2.1.3), the Near-Field Region (Figure 4-6 and Sections 4.2.1.4 through 4.2.1.6), the Far-Field Region (Figure 4-7 and Sections 4.2.1.7 and 4.2.1.8), the Biosphere Region (Section 4.2.1.9), and the fast pathway (Section 4.1.1.10).

To simulate a specific disposal system alternative using GPAM, appropriate system-level specifications must be made (Section 4.2.1.1) and each of the disposal system features/components/regions must be associated with one or more GPAM domains. Parameter values (geometry, solid, fluid, transport, and fracture, if needed) can then be selected for each GPAM domain such that it represents the specific engineered material or geologic media of the disposal system feature/component/region of interest.

Although the eight GPAM domains are intended to correspond to specific disposal system features (Figure 4-3), there is no restriction against using a specific model domain to represent something different. Each model domain is simply a combination of one or more GoldSim transport elements (cells and/or pipes), therefore, any feature/component/region of a disposal system can be represented by any transport element (keeping in mind that GoldSim cells better represent diffusive-dominated transport and GoldSim pipes better represent advective-dominated transport). For example, the EBS Outer domain could be used to represent a host rock geologic medium.

In GPAM V0 all eight GPAM domains need to be present and parameterized in each disposal system simulation. However, it should be noted that the EBS Inner and EBS Outer model domains provide identical capabilities (i.e., a three-cell transport pathway, with or without dual porosity) and the Near-Field Host Rock and Far-Field Host Rock model domains provide identical capabilities (i.e., a five-pipe or five-cell transport pathway). Therefore, it is easy to consolidate the EBS into an equivalent single six-cell transport pathway by giving both the EBS Inner and EBS Outer model domains identical input parameter values. Similarly, the Host Rock can be consolidated into an equivalent single ten-cell transport pathway. Additionally, a GPAM model domain can be implicitly by-passed through the use of appropriate parameterizations if that model domain is not needed for a specific simulation. The capability to explicitly bypass or de-activate model domains will be added in a future version.

It should also be noted that, in GPAM V0, all elements in a multi-element model domain must have the same geometry. For example, in a 5-pipe Far-Field Host Rock, the total domain volume and total domain transport length as specified as input parameters. Each pipe is then automatically assigned 1/5 of those values. The capability to specify variable element geometries, and possibly even a variable number of elements, within a model domain will be added in a future version.

Table 4-3. Conceptualization of GPAM Domains in GoldSim

GPAM Domain	GPAM Domain and GoldSim Transport Elements	Summary Description[a]
System Level	Repository Configuration	Number of transport pathways Number of waste packages (total and per pathway) Fast Pathway flag (present / not present)
	Radionuclide Species	Atomic weight Half life Specific activity Decay chains
	Radionuclide Inventory	Radionuclide mass per waste package
	Reference Temperature[b]	Reference temperature
	Reference Fluid Properties[c]	Reference (i.e., free water) diffusivity Radionuclide relative diffusivities Radionuclide solubilities
	Property Libraries	Inventory Diffusion (diffusion coefficients) Solubility Sorption (distribution coefficients) Dose factors
Source Term	Degraded Waste Form • 1 Source (Waste Degradation) • 1 Cell (Degraded Waste Form)	Waste form degradation rate Waste package failure time Domain geometry[d] Domain solid (WF_Debris) properties[e] Domain fluid properties[f] Domain transport properties[g]
	Degraded Waste Package • 1 Cell (Degraded Waste Package)	Domain geometry[d] Domain solid (WP_Debris) properties[e] Domain fluid properties[f] Domain transport properties[g]
Near Field	EBS Inner • 3 Cells (EBSInner_1 to _3) • 3 Cells (EBSInner_1F to _3F) (Cells _1F to _3F represent fractures if dual porosity is specified for this domain)	Dual porosity flag (no fractures / fractures) Domain geometry[d] Domain solid (EBSInner_Medium) properties[e] Domain fluid properties[f] Domain fracture properties (if needed)[h] Domain transport properties[g]
	EBS Outer • 3 Cells (EBSOuter_1 to _3) • 3 Cells (EBSOuter_1F to _3F) (Cells _1F to _3F represent fractures if dual porosity is specified for this domain)	Dual porosity flag (no fractures / fractures) Domain geometry[d] Domain solid (EBSOuter_Medium) properties[e] Domain fluid properties[f] Domain fracture properties (if needed)[h] Domain transport properties[g]
	Near-Field Host Rock • 5 Pipes (Adv1 to 5) OR • 5 Cells (Diff1 to 5) OR • 2D 20x20 Cell network (Pipes for advective-dominated transport, Cells for diffusive-dominated transport)	Dimension flag (1D / 2D)[i] Transport type flag (advective / diffusive) Domain geometry[d] Domain solid (NF_HostRock_Medium) properties[e] Domain fluid properties[f] Domain transport properties[g] Domain fracture properties (if needed)[h]

Table 4-3. Conceptualization of GPAM Domains in GoldSim (continued)

GPAM Domain	GPAM Domain and GoldSim Transport Elements	Summary Description[a]
Far Field	Far-Field Host Rock • 5 Pipes (Adv1 to 5) OR • 5 Cells (Diff1 to 5) OR • 2D 20x20 Cell network (Pipes for advective-dominated transport, Cells for diffusive-dominated transport)	Dimension flag (1D / 2D)[i] Transport type flag (advective / diffusive) Domain geometry[d] Domain solid (FF_HostRock_Medium) properties[e] Domain fluid properties[f] Domain transport properties[g] Domain fracture properties (if needed)[h]
	Aquifer • 1 Pipe (Aquifer_Pipe)	Domain geometry[d] Domain solid (Aquifer_Medium) properties[e] Domain fluid properties[f] Domain transport properties[g] Aquifer transverse spreading factor [j]
Biosphere	Receptor	Radionuclide mass flux (g/yr) from Aquifer Domain Radionuclide specific activity (Bq/g) from RN Species Radionuclide Dose coefficients (Sv/Bq) (ERB1) Water consumption rate (ERB1 = 1.2 m3/yr) Dilution (pumping) rate (ERB1 = 10,000 m3/yr)
Fast Path[k]	Fast Pathway • 1 Source (Fast Path Source) • To-Be-Determined (TBD) Cells and/or Pipes	TBD[k]

NOTE: [a] GPAM V0 assumes all parameter values are constant over the entire duration of the simulation. The capability for time-varying parameter values will be added in a future version.

[b] GPAM V0 assumes all simulations are isothermal. The specification of some parameter values (e.g., solubility, sorption) may consider temperature, but temperature is not an input parameter. The capability for explicit temporal and spatial specification of temperature, and the corresponding dependence of other parameter values on temperature, will be added in a future version.

[c] Reference fluid properties represent default values. Domain-specific fluid properties may be specified to account for local differences (i.e., due to spatial variations in temperature or fluid chemistry).

[d] Domain geometry includes: volume, transport length, cross-sectional area (perpendicular to transport), and perimeter (perpendicular to transport).

[e] Domain solid properties include: bulk density, porosity, tortuosity, radionuclide distribution coefficients (sorption), and radionuclide available porosities.

[f] Domain fluid properties include: radionuclide relative diffusivities (if different from the reference fluid) and radionuclide solubilities.

[g] Domain transport properties include: source zone length, volumetric flow rate, and dispersivity.

[h] Domain fracture properties include: spacing and aperture. Matrix diffusion parameters will be added in a future version.

[i] The Dimension flag allows for the selection of either a 1D transport pathway (a series of Pipes or Cells) or a 2D transport pathway (a cell network).

[j] The Aquifer transverse spreading factor accounts for "spreading" of radionuclides transverse to the transport pathway cross-sectional area (Section 4.2.1.8). It is applied at the interface between the FF Host Rock and Aquifer domains.

[k] The Fast Path capability is not functional in GPAM V0. It will be added in a future version.

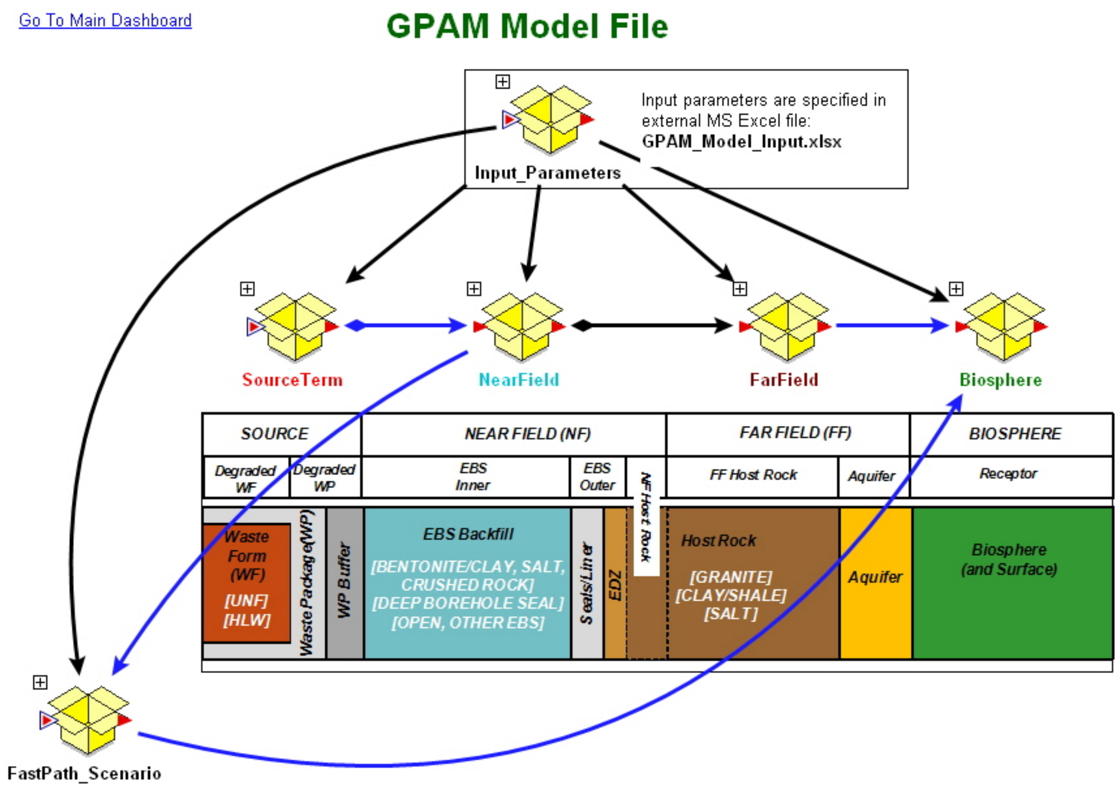


Figure 4-4. GPAM GoldSim Model File

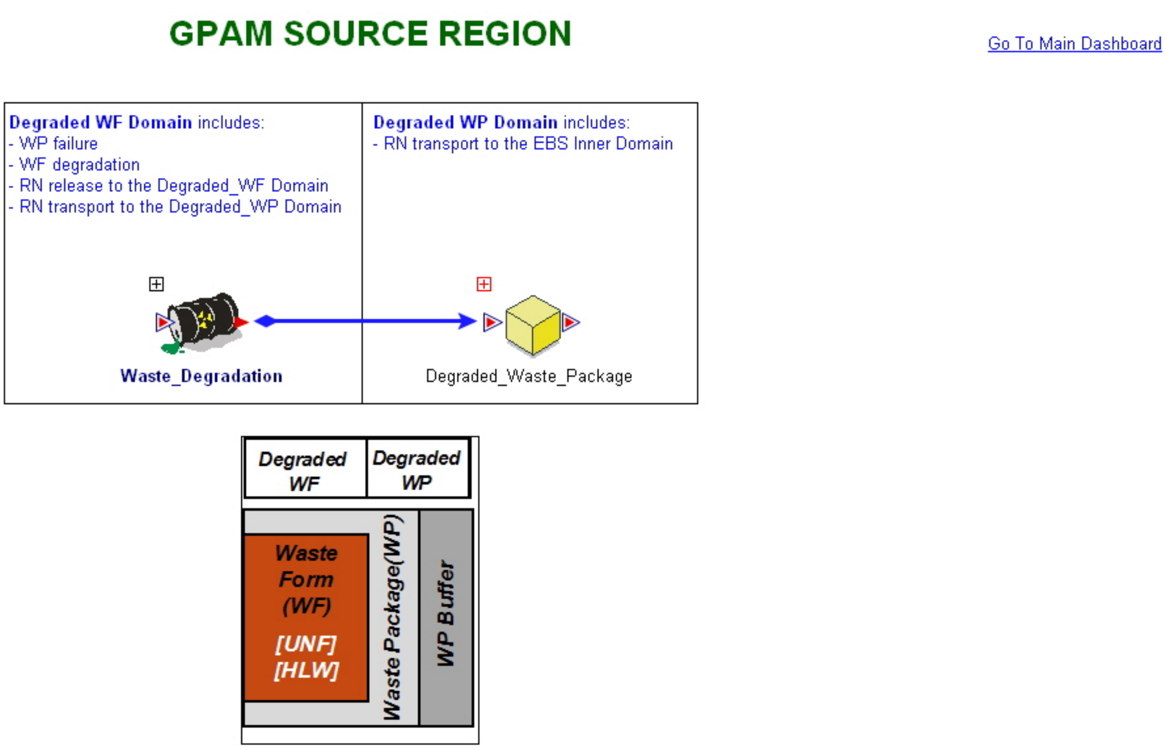


Figure 4-5. GoldSim GPAM Source Region

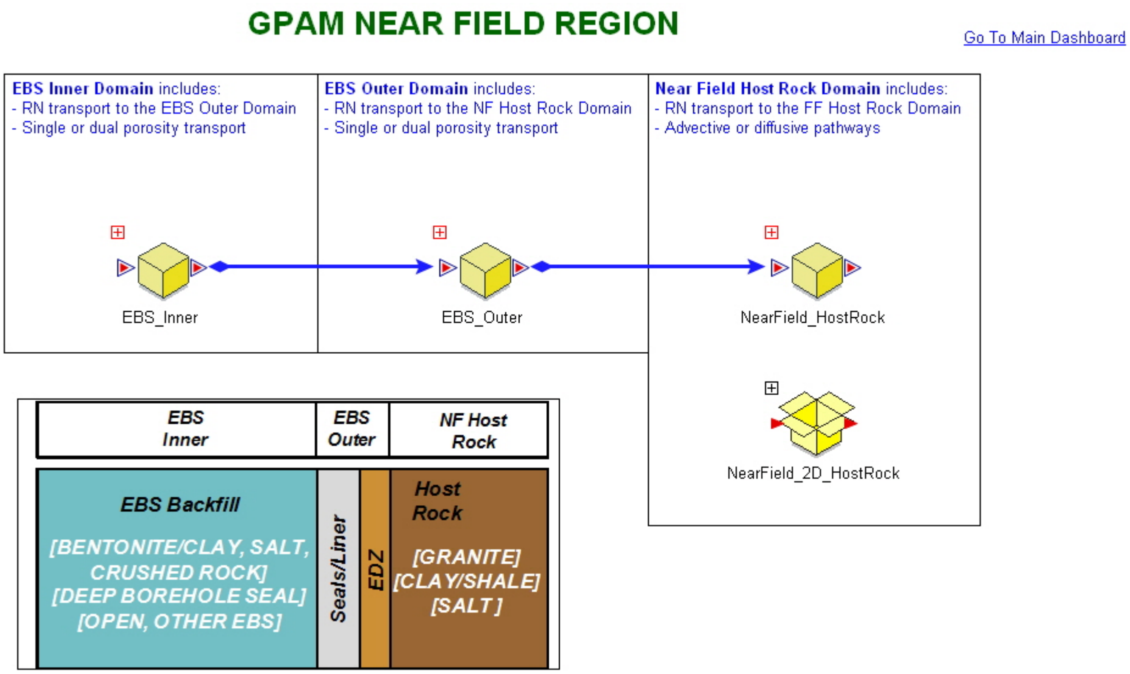


Figure 4-6. GoldSim GPAM Near Field Region

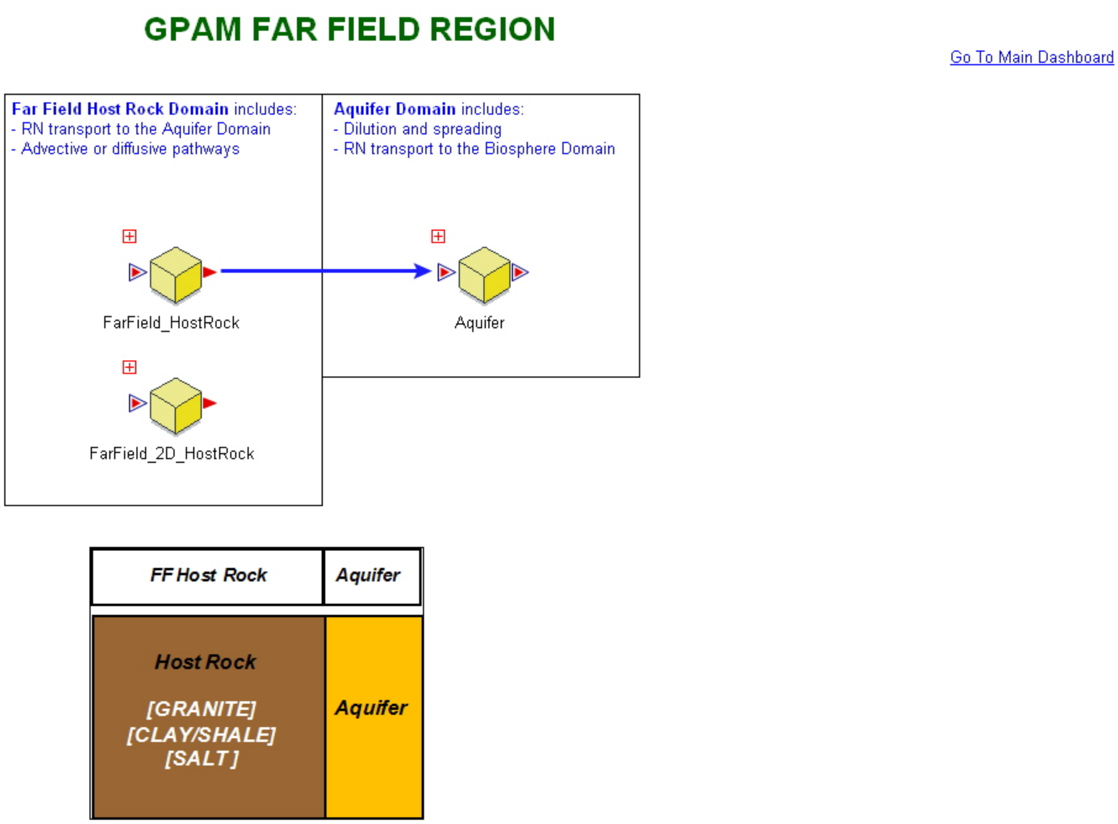


Figure 4-7. GoldSim GPAM Far-Field Region

4.2.1.1 System-Level Specifications

System-level specifications include system configuration, radionuclide species and properties, initial radionuclide inventory, temperature, reference fluid properties, and libraries of properties that may be used in the characterization of the eight model domains (e.g., solubility, sorption, diffusivity, and dose factors). The system-level specifications are described in the following paragraphs. Specific system-level input parameters are identified in Section 4.2.2.

Repository Configuration—The basic GPAM simulation unit is a transport pathway. The GPAM domains describe a single GPAM transport pathway from the source (which may contain 1 or more waste packages) to the receptor. This is illustrated schematically in Figure 4-8.

GPAM has the capability to account for multiple transport pathways. In GPAM V0 each transport pathway is assumed to have identical characteristics. As a result, a multiple pathway simulation simply applies a multiplier to the single pathway result. This capability is illustrated schematically in Figure 4-8, which identifies ten parallel GPAM transport pathways at the Far Field – Aquifer interface. The capability to simulate multiple GPAM transport pathways with different inventories and/or characteristics will be explored in future versions.

As illustrated in Figure 4-8, the GPAM transport pathway has a cross-sectional area perpendicular to the longitudinal direction of transport. In the GPAM the cross-sectional area of transport is defined strictly as an area (i.e., it does not necessarily have a length, width, or radius), so it can represent any geometry.

However, the longitudinal dimension of the GPAM transport pathway (e.g., the distance from Source Term to Biosphere) is typically much longer than the cross-sectional/transverse dimensions. As a result, the transport pathway is essentially 1D, consistent with Equation 4-23, which only includes longitudinal spreading (mechanical dispersion and diffusion in the D_x term). To include the effects of transverse spreading beyond the dimensions of the GPAM transport pathway cross-section (e.g., a quasi-3D geometry), a transverse spreading factor can be specified (Section 4.2.1.8).

Radionuclide Species—Each radionuclide is defined by a half-life, atomic weight, and specific activity. Parent-daughter relationships are also defined through the specification of decay chains.

Radionuclide Inventory Library—Radionuclide inventory information are contained in the Inventory Library. The Inventory Library may contain multiple user-specified inventories, with each inventory quantifying the initial mass of each radionuclide per waste package. Differences between inventories reflect differences in waste form type, aging, etc.

Temperature— GPAM V0 assumes all simulations are isothermal. The specification of some parameter values (e.g., solubility, sorption) may consider temperature, but temperature is not an input parameter. The capability for explicit temporal and spatial specification of temperature, and the corresponding dependence of other parameter values on temperature, will be added in a future version, once the EBS architecture is further refined (Section 5).

Reference Fluid Properties—Each fluid is defined by a reference diffusivity, and relative diffusivities and solubilities for each radionuclide. The reference fluid provides default properties throughout the model. If fluid properties within a model domain are different from the reference properties, they can be specified within that domain.

Property Libraries—Information describing solubility, sorption, diffusion, and dose factors are contained in property libraries. Each of these libraries may contain multiple sets of parameter values representative of different media and/or fluid types.

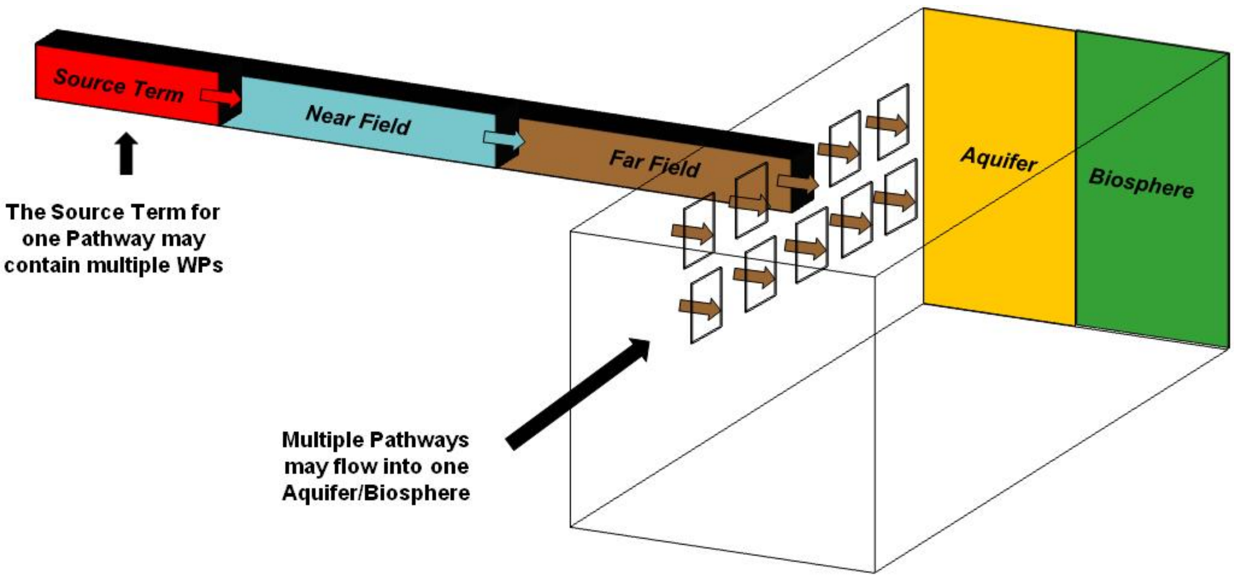


Figure 4-8. Schematic Representation of a GPAM Transport Pathway

4.2.1.2 Degraded Waste Form Domain

The Waste Form domain consists of a Degraded_Waste_Form container inside of a Waste_Degradation Source element (Figure 4-5). Within the Waste_Degradation Source element, the initial radionuclide inventory, waste form degradation rates, and waste package failure times are specified. In GPAM V0 the entire radionuclide mass that is mobilized from the waste form is assumed to be dissolved in water in the pore space (or precipitated). The capability for colloidal radionuclides (formation and transport) and gas phase will be added in a future version. The GoldSim elements within the Degraded_Waste_Form container are shown in Figure 4-9. This model domain contains one transport element, the Degraded_WF cell. Dissolved radionuclides that are mobilized from the waste form move through the Degraded_WF cell. Solid properties are defined within the WF_Debris solid element.

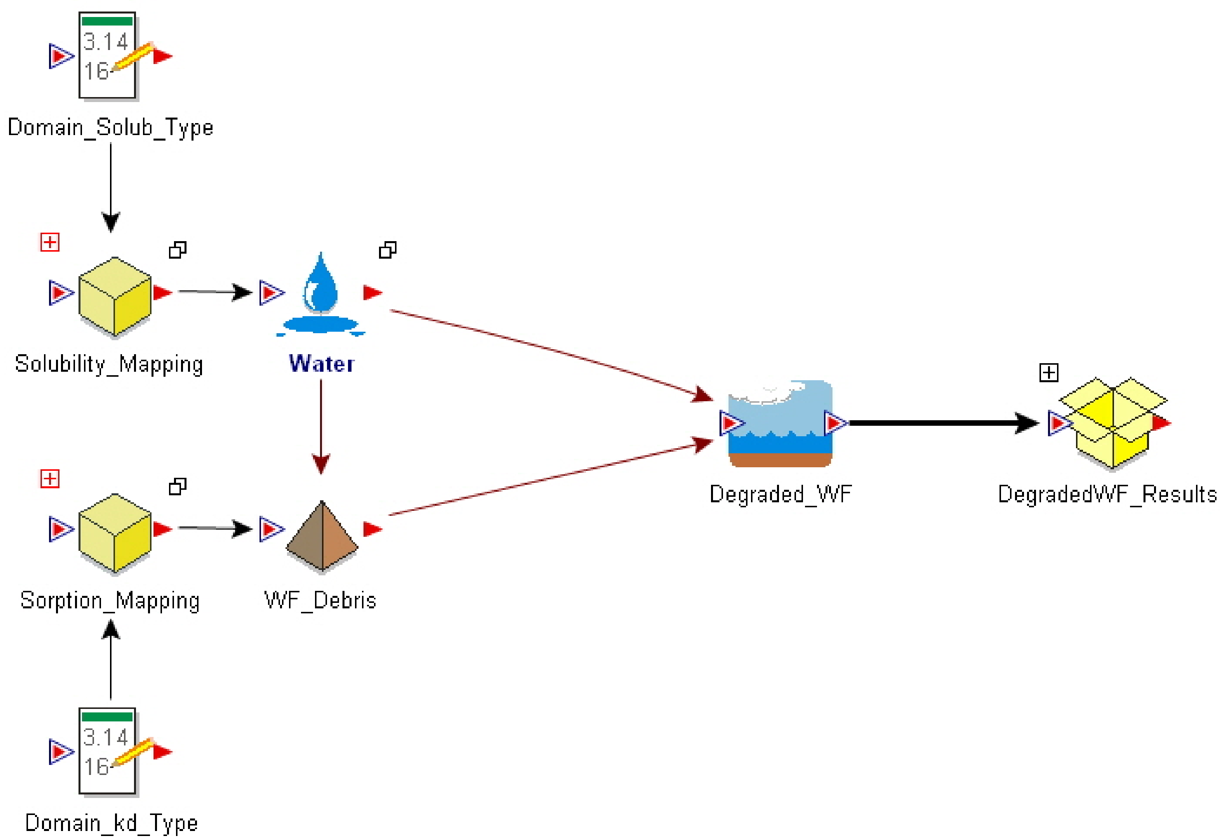


Figure 4-9. GoldSim GPAM Degraded Waste Form Domain Elements

4.2.1.3 Degraded Waste Package Domain

The GoldSim elements within the Degraded_Waste_Package container are shown in Figure 4-10. This model domain contains one transport element, the Degraded_WP cell. Dissolved radionuclides from the Degraded_WF cell move into and through the Degraded_WP cell. Solid properties are defined within the WP_Debris solid element.

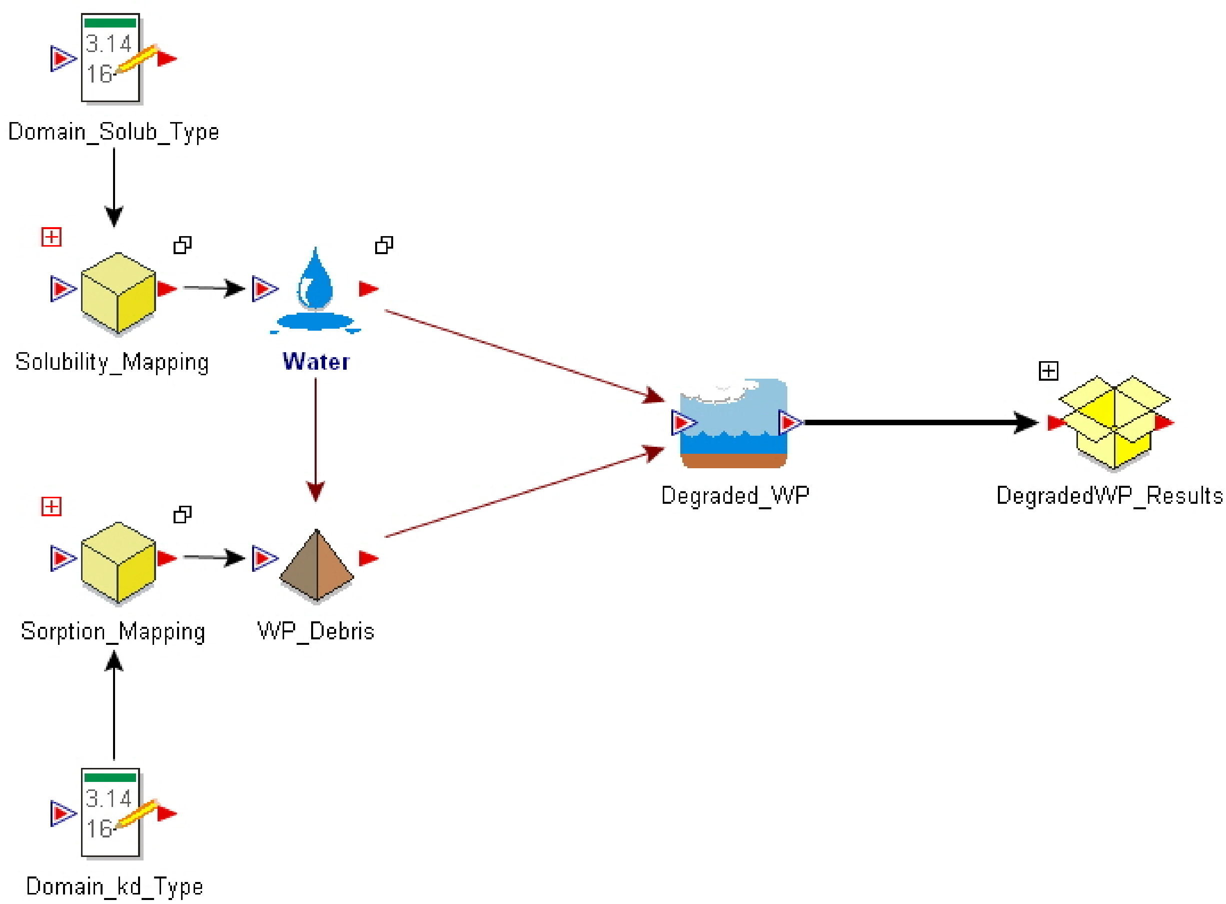
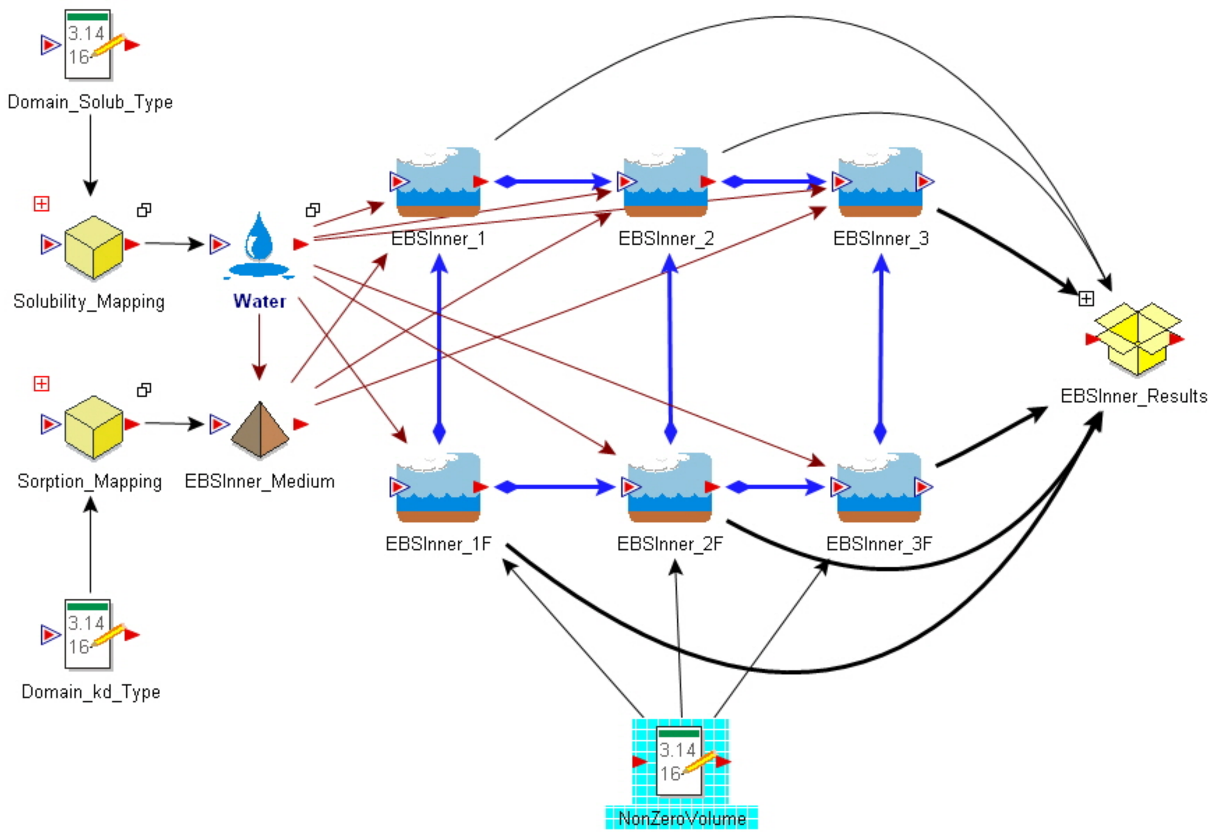


Figure 4-10. GoldSim GPAM Degraded Waste Package Domain Element

4.2.1.4 EBS Inner Domain

The GoldSim elements within the EBS_Inner container are shown in Figure 4-11. This model domain contains two parallel transport pathways, each containing three transport elements. For a single porosity conceptualization, only the three cells EBSInner_1 through EBSInner_3 are used and dissolved radionuclides from the Degraded_WP cell move into and through the three-cell transport pathway. For a dual porosity conceptualization, radionuclide transport is predominantly through the three cells EBSInner_1F through EBSInner_3F, which represent the fracture porosity. Cells EBSInner_1 through EBSInner_3 represent the matrix porosity. The specification of a single porosity or a dual porosity conceptualization is made using the input parameter EBSInner_DualPorFlag (Section 4.2.2 and Figure 4-19). Solid properties are defined within the EBSInner_Medium solid element.



NOTE: The NonZeroVolume element adds a small volume of water (0.1 m^3) to eliminate the error message of "zero volume for cells EBSInner_1F through EBSInner_3F" that occurs when the dual porosity cells are not active.

Figure 4-11. GoldSim GPAM EBS Inner Domain Elements

4.2.1.5 EBS Outer Domain

The GoldSim elements within the EBS_Outer container are shown in Figure 4-12. This model domain has the same conceptualization (single or dual porosity) and functionality as the EBS Inner domain (Section 4.2.1.4). The specification of a single porosity or a dual porosity conceptualization is made using the input parameter EBSOuter_DualPorFlag. Solid properties are defined within the EBSOuter_Medium solid element. Dissolved radionuclides from the EBS Inner domain (cell EBSInner_3 and/or cell EBSInner_3F) move into and through the EBS Outer domain cells.

Although, the EBS Inner and EBS Outer domains have the same functionality, different conceptual models (single or dual porosity) and different sets of parameter values can be assigned to each domain. Conversely, the same parameter values can be assigned to both domains, in which case they will collectively represent a single 6-cell (or 12-cell if dual porosity is specified) transport pathway.

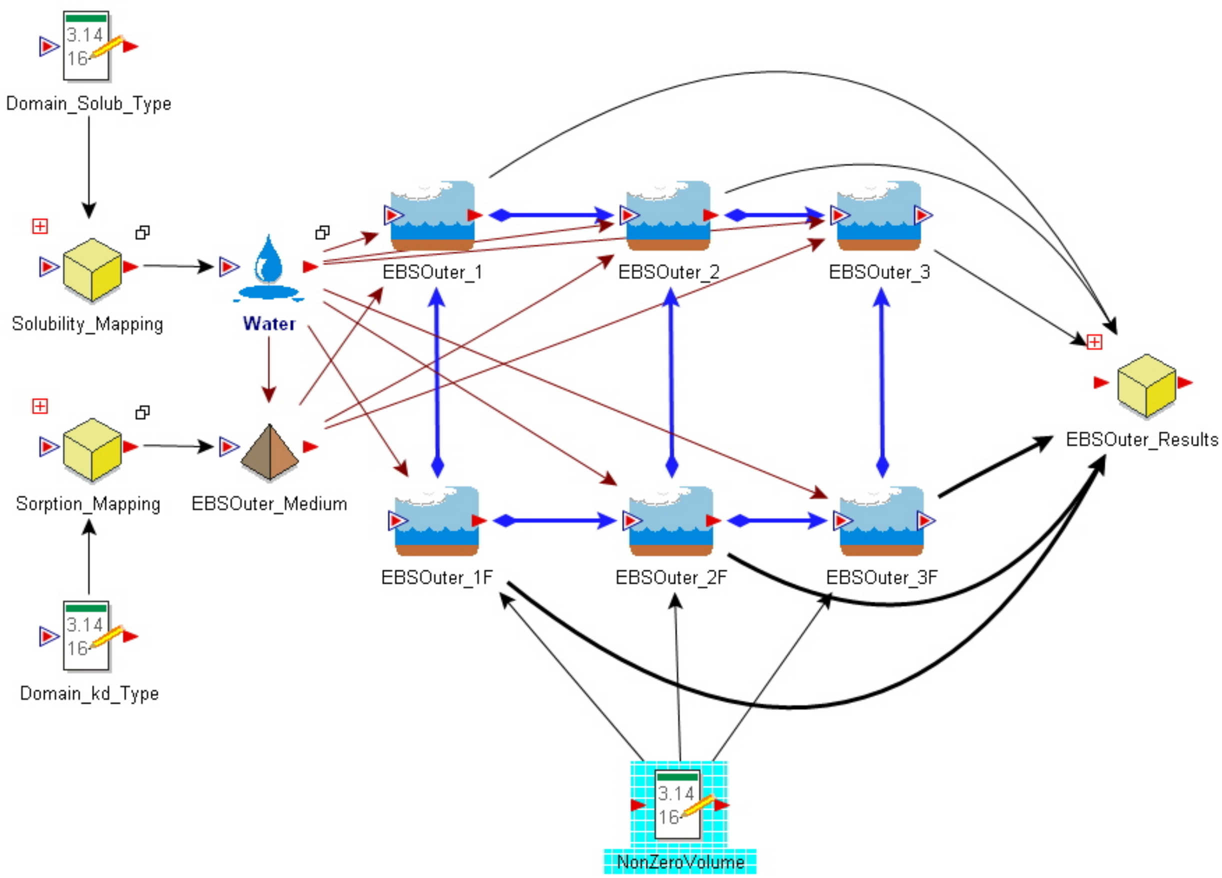
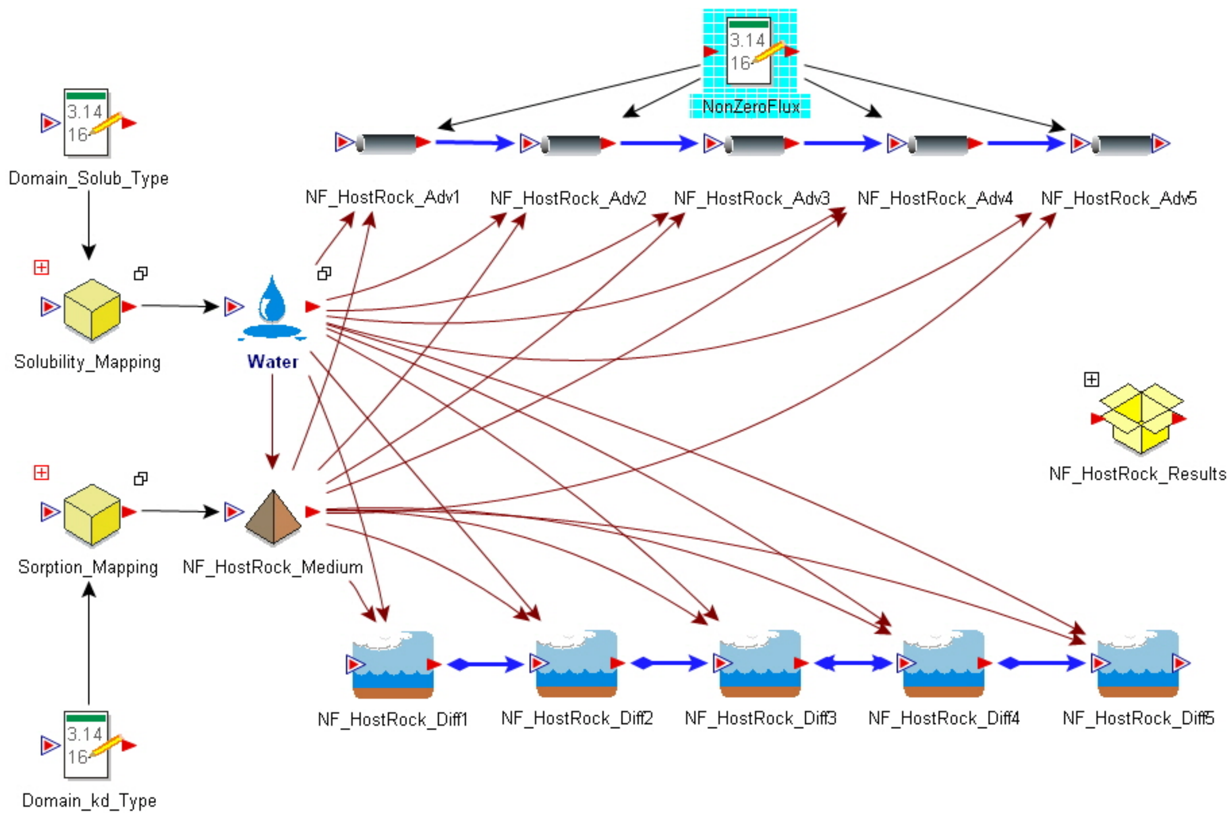


Figure 4-12. GoldSim GPAM EBS Outer Domain Elements

4.2.1.6 Near-Field Host Rock Domain

The Near-Field Host Rock domain can be conceptualized with either a 1D (quasi-3D) or 2D (quasi-3D) geometry. The 1D geometry is defined within NearField_HostRock container and the 2D geometry is defined within the NearField_2D_HostRock container (Figure 4-6). The selection of 1D or 2D geometry is made using the input parameter NFRock_1D2D. In GPAM V0 only the 1D geometry is available. The 2D geometry will be added in a future version.

The GoldSim elements within the NearField_HostRock container (i.e., for 1D geometry) are shown in Figure 4-13. This model domain contains two independent transport pathways, each containing five transport elements. For advective-dominated transport, only the five pipes NF_HostRock_Adv1 through NF_HostRock_Adv5 are used and dissolved radionuclides from the EBS Outer domain (cell EBSOuter_3 and/or cell EBSOuter_3F) move into and through the five-pipe transport pathway. For diffusive-dominated transport, only the five cells NF_HostRock_Diff1 through NF_HostRock_Diff5 are used and dissolved radionuclides from the EBS Outer domain move into and through the five-cell transport pathway. The specification of an advective- or diffusive-dominated transport conceptualization is made using the input parameter NFRock_TranType. Solid properties are defined within the NF_HostRock_Medium solid element.



NOTE: The NonZeroFlux element adds a small lux of water (1×10^{-50} m^3/yr) to eliminate the error message of "zero flow rate in Pipes NF_HostRock_Adv1 through NF_HostRock_Adv5" that occurs when the cells (diffusive-dominated transport) are utilized.

Figure 4-13. GoldSim GPAM Near-Field Host Rock Domain Elements

4.2.1.7 Far-Field Host Rock Domain

The Far-Field Host Rock domain can be conceptualized with either a 1D (quasi-3D) or 2D (quasi-3D) geometry. However, as with the Near-Field Host Rock domain, only the 1D geometry is available in GPAM V0. The 2D geometry will be added in a future version.

The GoldSim elements within the FarField_HostRock container (i.e., for 1D geometry) are shown in Figure 4-14. This model domain has the same conceptualization and functionality (5 pipes for advective-dominated transport or 5 cells for diffusive-dominated transport) as the Near-Field Host Rock domain (Section 4.2.1.6). The specification of an advective- or diffusive-dominated transport conceptualization is made using the input parameter FFRock_TranType. Solid properties are defined within the FF_HostRock_Medium solid element. Dissolved radionuclides from the Near-Field Host Rock domain (pipe NF_HostRock_Adv5 or cell NF_HostRock_Diff5) move into and through the specified Far-Field Host Rock domain transport pathway.

Although, the Near-Field Host Rock and Far-Field Host Rock domains have the same functionality, different conceptual models (advective-dominated or diffusive-dominated) and different sets of parameter values can be assigned to each domain. Conversely, the same parameter values can be assigned to both domains, in which case they will collectively represent a single 10-element transport pathway.

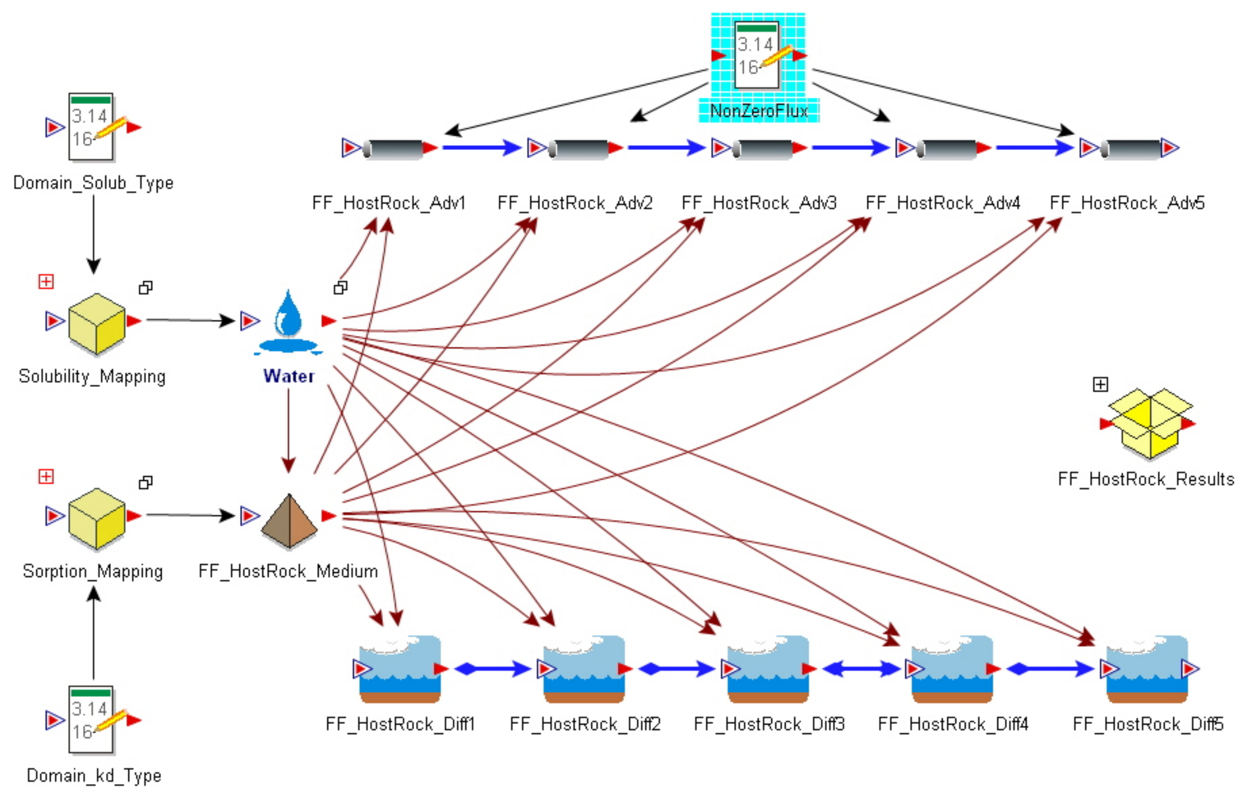


Figure 4-14. GoldSim GPAM Far-Field Host Rock Domain Elements

4.2.1.8 Aquifer Domain

The GoldSim elements within the Aquifer container are shown in Figure 4-15. For GPAM V0 this model domain contains one transport element, the Aquifer_Pipe pipe. A second transport element, the FarField_2D_HostRock_Collector cell, will be implemented in a future version, once the capability for 2D geometry has been added to the Near-Field and Far-Field Host Rock domains (Sections 4.2.1.6 and 4.2.1.7). Dissolved radionuclides from the Far-Field Host Rock domain (pipe FF_HostRock_Adv5 or cell FF_HostRock_Diff5) move into and through the Aquifer_Pipe pipe. Solid properties are defined within the Aquifer_Medium solid element.

As described in Section 4.2.1.1, the GPAM mathematical representation of the transport pathway only includes longitudinal spreading. To include the effects of transverse spreading beyond the dimensions of the transport pathway cross-section, a transverse spreading factor, D_{TS} , can be applied:

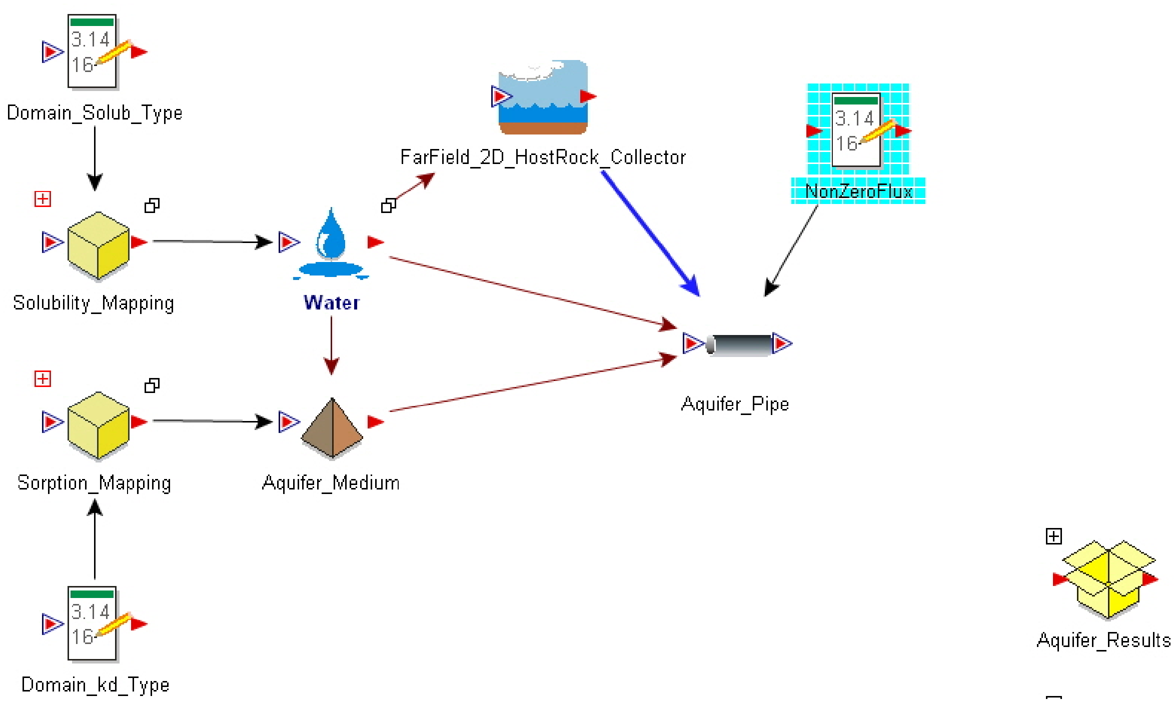
$$D_{TS} = \frac{A_{TS}}{A_P} \qquad \text{Eq. 4-29}$$

where:

A_P = cross-sectional area of the transport pathway [L^2]

A_{TS} = cross-sectional area of transport with transverse spreading [L^2]

The transverse spreading factor, if specified, is applied at the interface between the Far-Field Host Rock and Aquifer domains.



NOTE: The NonZeroFlux element adds a small flux of water (1×10^{-50} m^3/yr) to eliminate the error message of "zero flow rate in Pipe Aquifer_Pipe" that can occur for certain conditions.

Figure 4-15. GoldSim GPAM Aquifer Domain Elements

4.2.1.9 Receptor Domain

The GoldSim elements within the GPAM Biosphere Region, which corresponds to the Receptor domain, are shown in Figure 4-16. As described in Section 4.1.1.3, The GPAM dose calculation is based on the IAEA BIOMASS ERB 1B dose model (Equation 4-28). Dissolved radionuclides from the Aquifer_Pipe provide the radionuclide mass flux to the receptor. Receptor parameter values, dilution rate and water consumption rate, are defined in Biosphere input elements (Section 4.2.2 and Figure 4-17). ERB1 dose coefficients are selected from the Dose Factor Library (Section 4.2.2 and Figure 4-18).

4.2.1.10 Fast Path

A fast path can be used to bypass one or more of the GPAM domains, such as to represent a human intrusion, or a seismic or igneous disruption. The fast pathway capability is not functional in GPAM V0, but will be added to a future version.

4.2.1.11 Results

There are a number of Results containers present in GPAM (see the Main Dashboard in Figure 4-2 and within each model domain in Figures 4-9 through 4-16). In GPAM V0 these containers are not functional. However, the capability to capture simulation results in these containers and export simulation results to external files will be added to a future version.

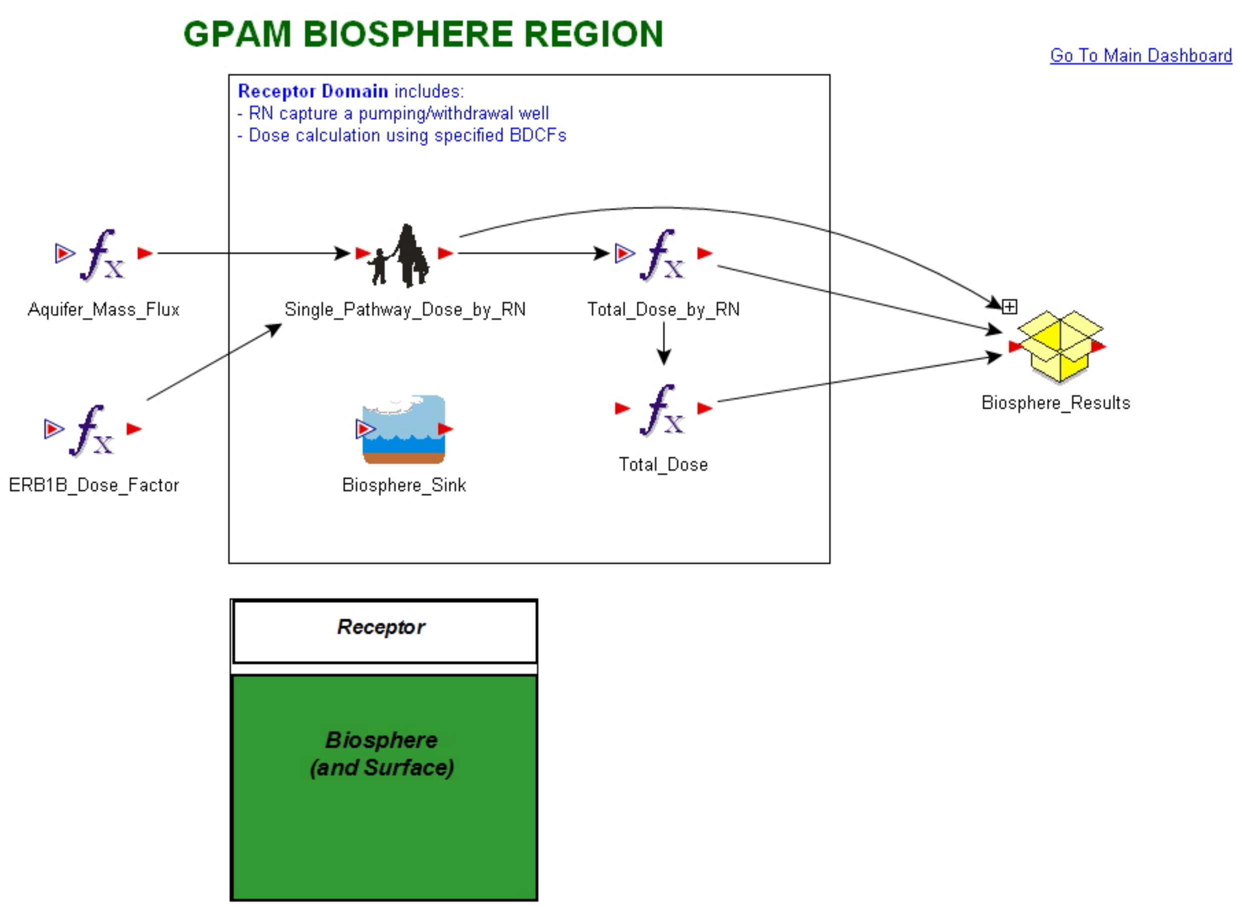


Figure 4-16. GoldSim GPAM Biosphere Region

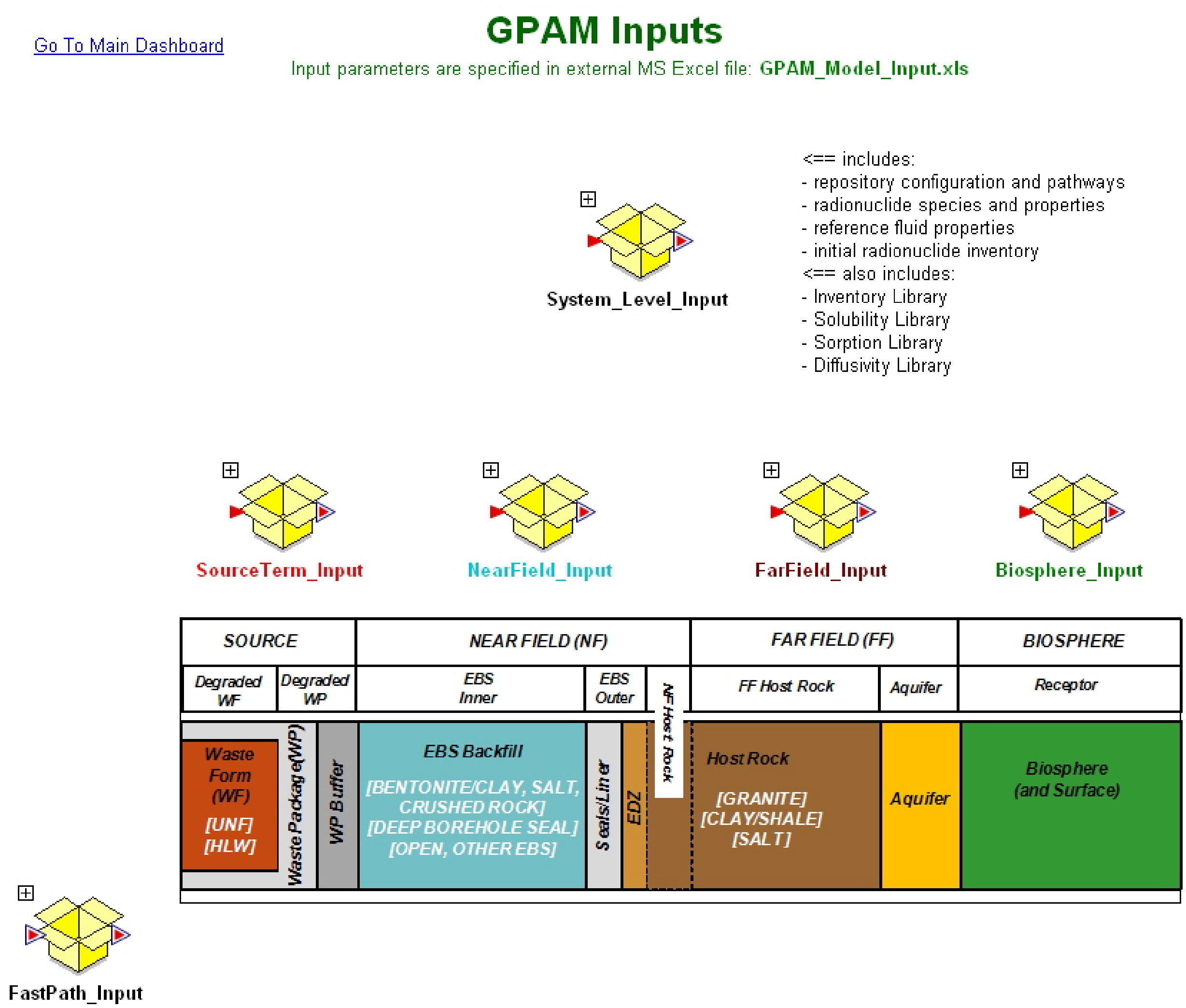


Figure 4-17. GoldSim GPAM Input Structure

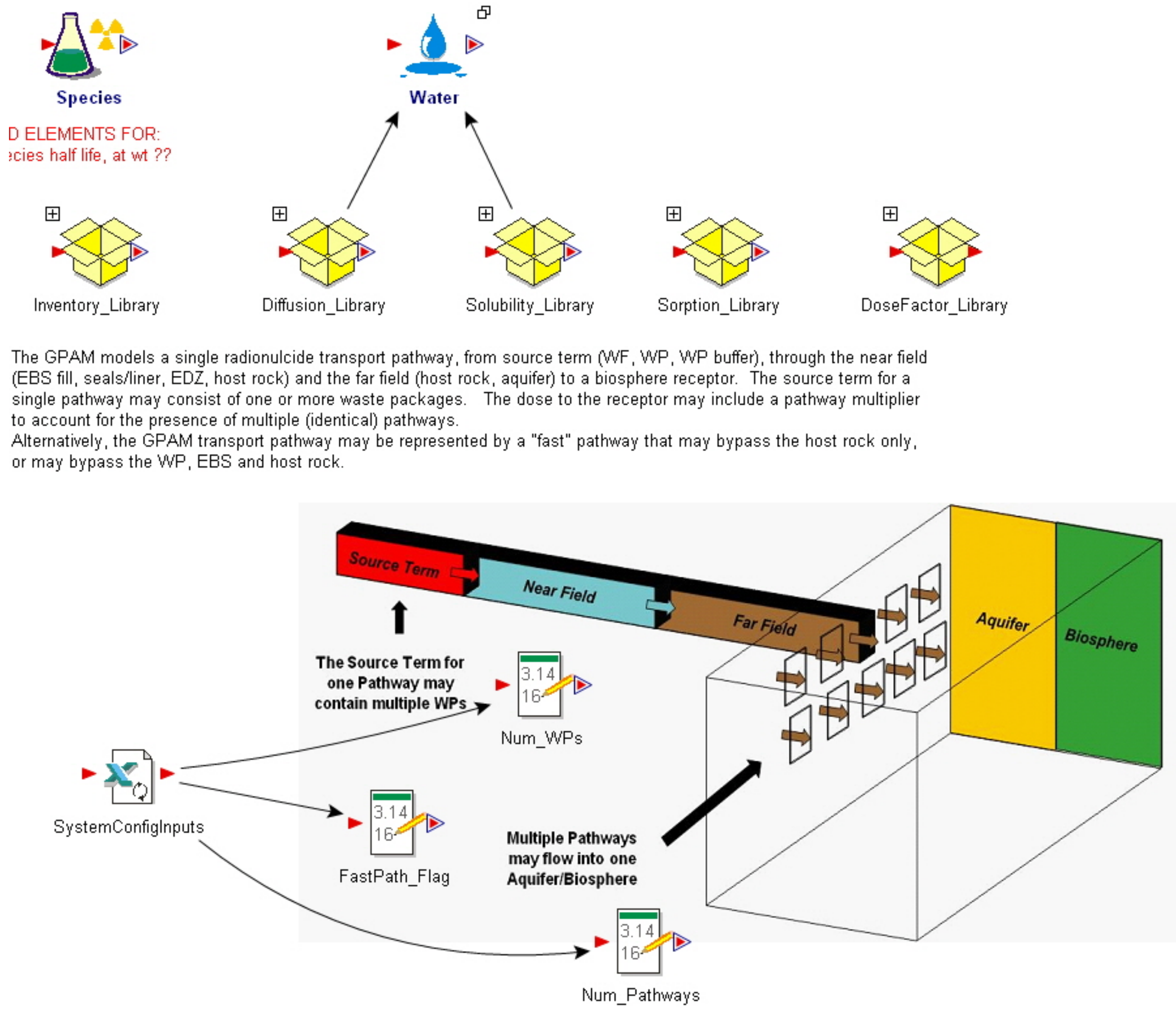


Figure 4-18. GoldSim GPAM System-Level Input Elements

4.2.2 GPAM Input Framework

Within GPAM, all input parameters are defined in the Input_Parameters container (Figure 4-4). Within the Input_Parameters container there are additional containers corresponding to the System_Level_ Inputs and to the GPAM region inputs (Figure 4-17). Each of the GPAM region input containers is further sub-divided by GPAM domain. The actual GPAM input elements are located within the System_Level_Inputs container and the eight GPAM domain input containers.

The GoldSim elements within the System_Level_Input container (Figure 4-18) are used to define values for the system-level parameters identified in Table 4-3 and discussed in Section 4.2.1.1. System-level parameters related to system configuration, radionuclide species and properties, initial radionuclide inventory, temperature, reference fluid properties, and the property libraries (solubility, sorption, diffusivity, and dose factors) are identified below. In addition the GoldSim simulation setting parameters are also identified below.

Repository Configuration—As described in Section 4.2.1.1, the GPAM V0 simulates radionuclide movement through a single transport pathway. The source term for a single GPAM transport pathway may contain multiple waste packages. System-level configuration parameters include the following: number of GPAM transport pathways, number of waste packages in a single pathway, and a flag to identify whether or not a Fast Path bypass is present. Parameters defining the geometry of the GPAM transport pathway (longitudinal distance, cross-sectional area, volume) are specified as part of the input parameters for each of the eight model domains.

Radionuclide Species—In GPAM V0 parameters defining the radionuclide species (decay chains, half-lives, atomic weights, specific activities) are hard-wired into the Species element. The capability to specify parameter values for radionuclide species external to GoldSim (e.g., in an MS Excel input file or parameter database) will added in a future version.

Initial Radionuclide Inventory—The initial inventory for a given simulation is selected from the Radionuclide Inventory Library. In GPAM V0 the initial inventory is limited to a single inventory from the Inventory Library and is defined by the mass of each radionuclide in a single waste package. GoldSim calculates the total inventory in a single GPAM transport pathway based on the number of waste packages per pathway and the per package inventory. The capability to specify (a) combinations (fractions) of different inventories, and (b) instantaneous release (i.e., gap and grain boundary) fractions will be added to future versions.

Temperature—In GPAM V0, temperature is not a direct input parameter. However, temperature-dependent parameters (e.g., sorption, solubility) may implicitly consider temperature by using values for a specific temperature or temperature range..

Reference Fluid Properties—Parameters defining the reference fluid (reference diffusivity, radionuclide relative diffusivities, and radionuclide solubilities) are specified within the Water fluid element. The radionuclide relative diffusivities and solubilities are selected from the Diffusion and Solubility Libraries, respectively. The Water element in the System_Level_Input container functions as the default fluid throughout the entire model. Clones of the Water element in each of the eight Model Domains provide the capability to specify local fluid properties that are different from the reference fluid.

Property Libraries—Parameters defining solubility, sorption, diffusion, and dose factors are contained in property libraries. Each of these libraries may contain multiple sets of parameter values representative of different media and/or fluid types. For a given simulation the specific property sets that apply to each model domain are defined as part of the input parameters for each of the eight model domains[e].

Simulation Settings—The GoldSim simulation setting parameters control the numerical solution to the simple mathematical representations identified in Section 4.1.1. Simulation parameters include time stepping, probabilistic sampling specifications, and solution precision. In GPAM V0 all simulation parameters are specified within GoldSim. The capability to specify the simulation parameters external to GoldSim (e.g., in an MS Excel input file or parameter database) will added in a future version.

Each of the eight GPAM domain input containers is used to specify parameter values that characterize the geometric, solid, fluid, fracture, and transport properties of the model domain. Additionally, source degradation properties are specified within the Waste Form model domain. Table 4-3 summarizes the types of properties that are required for each GPAM domain.

The GPAM domain input containers all have a similar architecture (i.e., they all contain similar elements and connections between elements), with the exception of the Biosphere input container. As an example, the input elements of the EBSInner_Input container are shown in Figure 4-19.

Figure 4-19 shows the specific parameters that are used to define EBS Inner model domain (and similarly, the other GPAM domains). These parameters are:

- *Geometric Properties*—Volume, TransportLength, Perimeter, Area (cross-sectional)[f], NumCells
- *Solid Properties*—BulkDensity, Porosity, Tortuosity, kd_Type, Available Porosity
- *Fluid Properties*—Solub_Type (if different from reference solubilities)
- *Fracture Properties*—DualPorFlag, Frac_Fraction, Frac_Spacing, Frac_Aperture, Frac_Area, Num_Fracs
- *Transport Properties*—Flow_Rate, Dispersivity

These input parameters are used to parameterize the fluid (Water), solid (EBSInner_Medium), and transport cells (EBSInner_1, etc.) within the EBS_Inner container (Figure 4-11) and similarly, other model domains. The capability to specify two additional fluid properties, saturation and radionuclide relative diffusivity, in each model domain will be added in a future GPAM version. Also, GoldSim pipes have the capability to simulate matrix diffusion. However, the specification of matrix diffusion parameter values (typically based on fracture properties) for pipes is not functional in GPAM V0. Therefore, matrix diffusion cannot be simulated in the Near-Field Host Rock, Far-Field Host Rock, and Aquifer domains in GPAM V0. The capability will be added to a future version.

In GPAM V0, most GoldSim input elements are fixed to accept either a deterministic value or a specified probability distribution. The capability to specify the type of distribution (or deterministic) externally will be added to a future version. The LHS DLL (Section 4.2.2.3) will contribute to this capability. Eventually, each input parameter may be specified as a single deterministic value or as a probability distribution.

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[e] Dose factors apply only to the Receptor model domain, solubility and sorption apply to the other seven model domains, and, for GPAM V0, diffusion only applies to the reference fluid.

[f] The cross-sectional area of the transport pathway should be the same across all model domains (except possibly the aquifer, if a transverse spreading factor is specified). Differences in the cross-sectional area between model domains could lead to unexpected changes in flow rates and/or concentrations (i.e., GoldSim may add or remove fresh water to maintain a water balance).

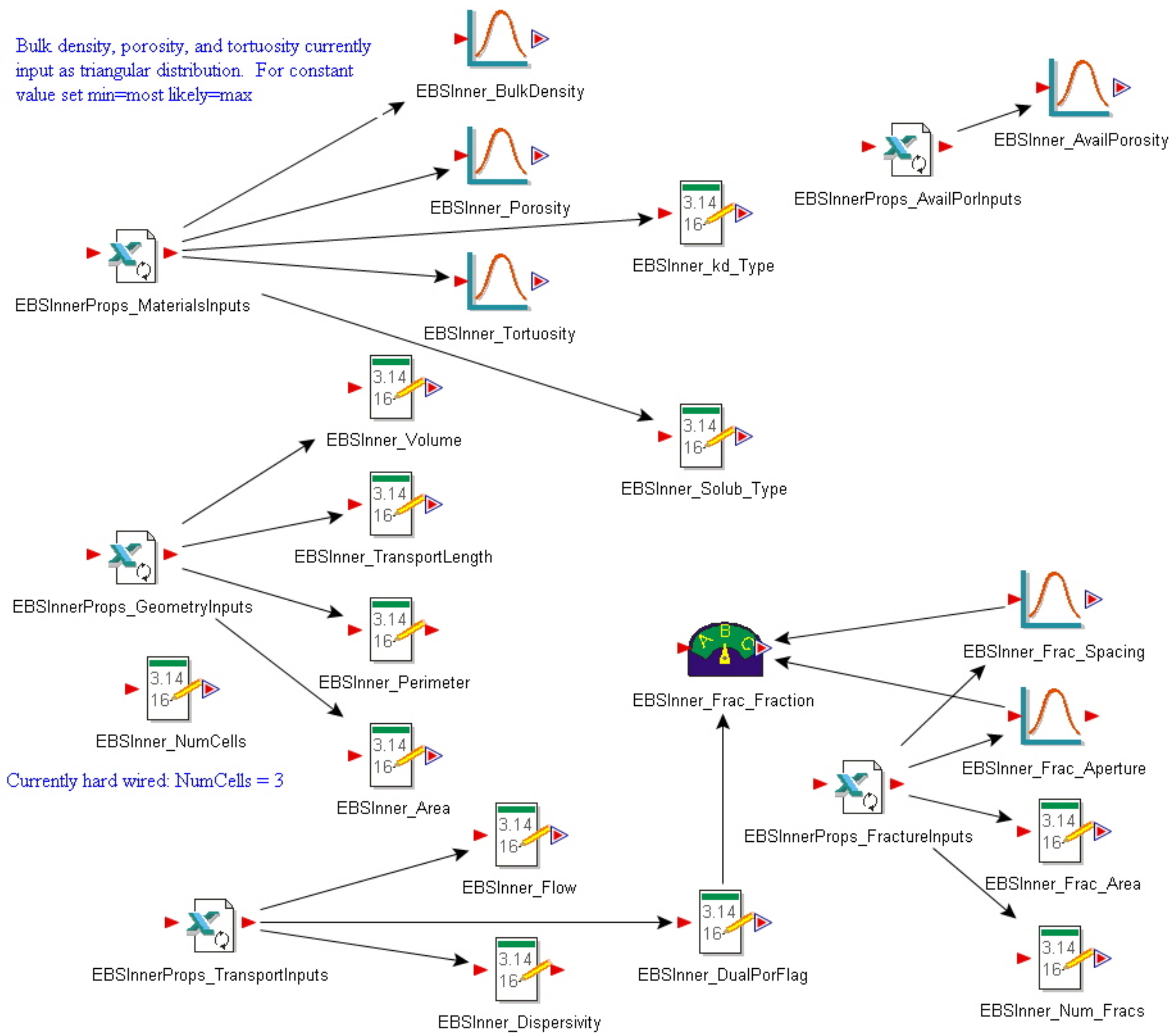


Figure 4-19. GoldSim GPAM EBS Inner Input Elements

In GPAM V0, the input elements obtain values (or distributions) from an external MS Excel spreadsheet (Section 4.2.2.1). In future versions, input values will come from an external relational database (Section 4.2.2.2).

4.2.2.1 MS Excel Spreadsheet

As noted in Section 4.2.2, GPAM V0 obtains values for input elements from an MS Excel spreadsheet. The MS Excel spreadsheet must have the name *GPAM_Model_Input.xlsx*. The MS Excel spreadsheet contains a number of worksheets including: GPAM_Overview, Table_of_Contents, a few corresponding to system-level parameters, several corresponding to each of eight model domains, and a few corresponding to the properties libraries (inventory, diffusion, solubility, sorption, and dose factors). In

GPAM V0, there is not a one-to-one mapping of worksheets to GoldSim GPAM domain input containers, but the mapping is still reasonably easy to trace. In future versions, this mapping will be more transparent.

As an example, the EBS_Inner_Properties worksheet is shown in Figure 4-20. These input values correspond to the input elements of the EBSInner_Input container as shown in Figure 4-19. In the worksheet in Figure 4-20:

- Column B provides values for deterministic parameters.
- Columns C through E provide values for probabilistic parameters
- Column F provides required units (these are units expected by GoldSim. While GoldSim itself can convert between like-dimensioned units, values coming into GoldSim from an external source cannot be converted.)
- Column G provides the distribution type. As noted earlier, GPAM V0 can only use pre-specified parameter distributions. In other words, the inputs are hard-wired to be deterministic (identified as scalar in Figure 4-20) or a specific probabilistic distribution (usually triangular). In future versions, column G will be used to specify the distribution externally (through integration with the LHS DLL described in Section 4.2.2.3).
- Column H identifies (with a “Y”) values that are directly input to GoldSim input elements
- Columns I and J provide rationale and/or reference information

The green highlighted cells represent values that need to be directly input. The unhighlighted boxes are values that are calculated from supporting inputs. Most of these supporting inputs are found in the worksheet rows below Row 36, labeled Supporting Calculations. The GPAM input elements require a constant set of inputs regardless of which disposal alternative is being simulated. For example, Row 21 requires a domain volume in m^3. However, depending on the conceptual model, the EBS Inner domain may in fact be a block or a cylinder. For a block, the volume is length × width × height, whereas for a cylinder, the volume is pi × diameter × height. To reduce potential complexity within GoldSim, these calculations need to be performed within the input spreadsheet and are defined in the Supporting Calculations rows of the worksheet.

Another example is volumetric flow rate (Row 26). The flow rate may in fact be calculated from hydraulic gradient and hydraulic conductivity, which in turn may be calculated from permeability, fluid density, fluid viscosity, and gravitational constant. However, all of these calculations would be defined in the Supporting Calculations.

In GPAM V0 the simulation settings, time-stepping, and model precision settings are hard-wired in GoldSim. In a future version these settings will be read in from the MS Excel spreadsheet (or the external database). It will also be desirable to add some sort of capability to perform checks on grid and time step size to avoid/minimize numerical errors in the solution or to increase numerical efficiency.

4.2.2.2 External Database

Eventually, the input parameter values will be input from an external relational database, rather than with the external MS Excel spreadsheet described in Section 4.2.2.1. However, the GoldSim input structure and elements (Section 4.2.2) will remain the same regardless of the input source. The external GDS Parameter Database is currently under development. The working requirements of the database have been completed. This subsection describes the planned development approach.

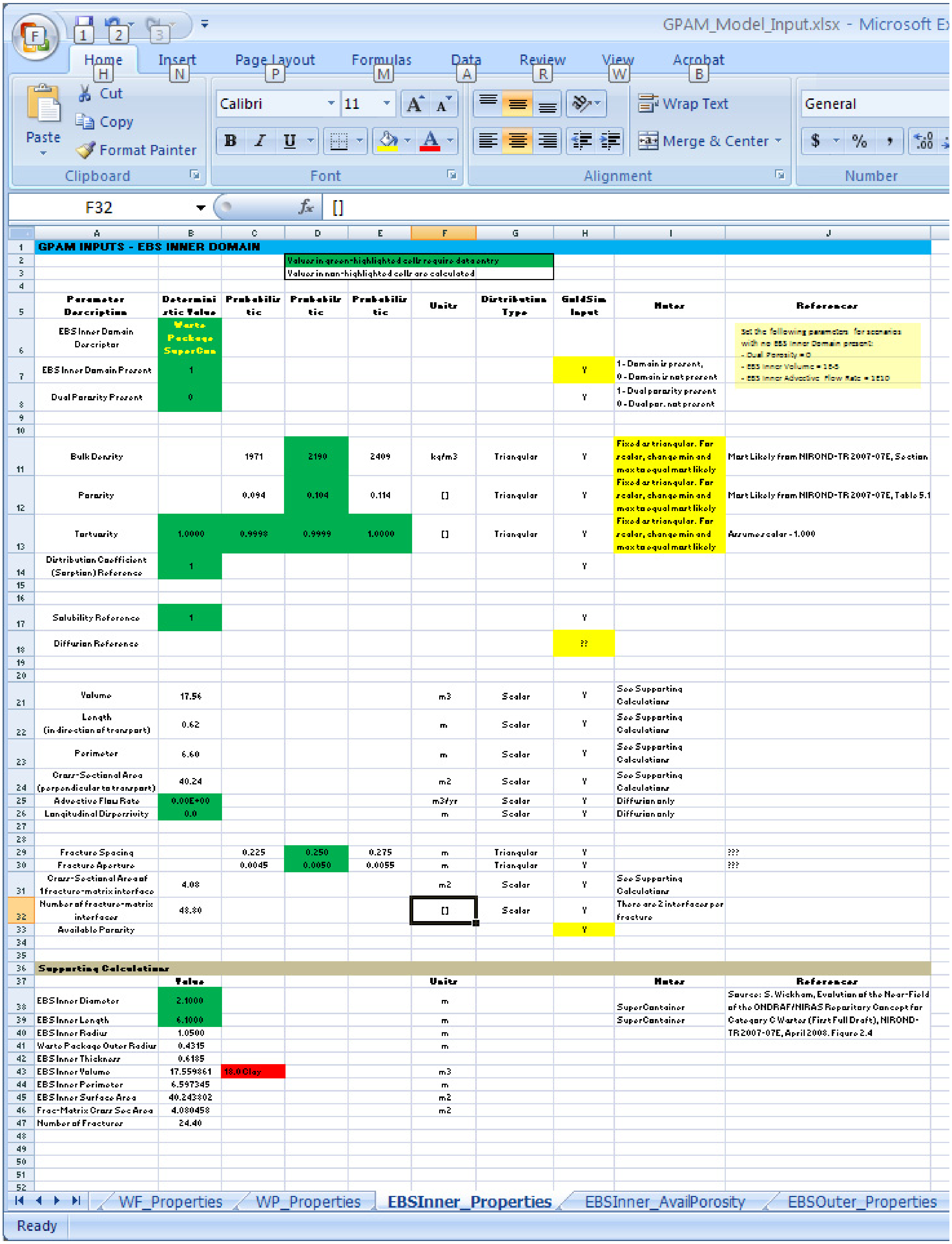


Figure 4-20. MS Excel Input File Worksheet EBSInner_Properties

The GDS Parameter Database will be a relational database that supports analyses of multiple disposal system alternatives using GPAM. The database will serve as the controlled source of parameter information for the GPAM calculations. The GDS Parameter Database will contain two types of parameter sets: GDS Parameters and GPAM Input Parameters.

The GDS Parameters include all of the data potentially relevant to all of the disposal system alternatives (e.g., solid properties representative a number of different geologies and engineered materials). Each GDS Parameter will be defined by information in a set of data fields, potentially including:

- Parameter Name
- Description
- Element Type (Data, Lookup Table, etc.)
- Distribution Type (Type_Code)
- Numerical Value(s)
- Units
- Disposal Alternative (geology, waste type, etc.)
- Model Domain (waste form, waste package, EBS, host rock, etc.)
- Parameter Type (geometry, fluid, solid, etc.)
- Notes/Discussion
- Links to the underlying basis
- Reference Document
- Effective Date
- Modification Date

These data fields include general information (data and GoldSim-specific information (e.g., Type_Code)) that a modeler will utilize. The breath of potential use for a specific GDS Parameter can be highly variable. Some GDS Parameters may be applicable to multiple disposal system alternatives and/or to multiple regions within a disposal system (e.g., solubility values). Other GDS Parameters may only be applicable to a single location/feature within a single disposal system alternative (e.g., sorption in a deep borehole seal). The Disposal Alternative and Model Domain data fields provide information to help the modeler understand the potential uses of the input data. Information on the underlying basis of input data allows the modeler to evaluate the information and to make an informed judgment on how it should be used. Modification date is important for maintaining version control (Section 4.2.3).

The GPAM Input Parameters define the values and/or probability distributions for a single GPAM simulation. The GPAM Input Parameters correspond directly to the GoldSim input elements identified in Section 4.2.2. For a specific GPAM simulation, a value (or distribution) for each GPAM Input Parameter will be selected from the GDS Parameters. The GPAM Input Parameters may be different for each simulation but are always selected from, and a subset of, the GDS Parameters. GDS Parameters will continue to be added to the database as new information becomes available (e.g., porosities for a specific type of clay, elemental solubilities for a specific chemical environment).

Once the set of GPAM Input Parameters has been specified for a specific GPAM simulation, they will be automatically input to the GPAM GoldSim input elements using protocols for external databases (e.g., Yucca Mountain Database protocols) described in the GoldSim User's Manual (GoldSim Technology

Group 2010c; Appendix F). Information to identify the set of GPAM Input Parameters used for a specific simulation will be stored in the GDS Parameter Database, with a unique identifier.

In conjunction with the configuration management protocols described in Section 4.2.3, the GDS Parameter Database will support and document the verification of the parameter information. It will also support production of a variety of reports that summarize information contained in the database.

4.2.2.3 Latin Hypercube Sampling DLL

The LHS DLL provides the capability to specify different parameter value distributions when using external input files (e.g., an MS Excel spreadsheet or an external database). The LHS DLL, based on original LHS software developed at SNL (Iman et al. 1980; Iman and Shortencarier 1984; Swiler and Wyss 2004), was developed to replace the internal sampling structure within GoldSim. DLLs are compiled libraries that can be called by software (e.g., GoldSim) to perform operations, such as an executable does, in the MS Windows® operating system. A DLL is used to perform calculations that cannot be done directly (or would take too much time and/or would be inefficient) with GoldSim elements alone. Further details on the LHS DLL and its implementation can be found in Sallaberry (2011).

To take uncertainty into account in GoldSim, a user can declare each variable as uncertain by selecting a stochastic element to represent it, associate a distribution with it (from the list of distributions available in the properties), and run a sample of desired size before computing statistics. There are, however, some limitations.

First, because of the way GoldSim generates random numbers, there is no assurance of the reproducibility of a sample. In GoldSim when a stochastic element is created, it is assigned its own unique (and internal, meaning not available to the developer) random seed. In other words, recreating an identical model with the same set of elements and using the same global random seed will have a different set of results because each element will have a different internal random seed. Moreover, if one erases a stochastic element and recreates it in the initial model, even with the same properties, the outcome will be a different sample at least for this element. The LHS DLL removes this limitation.

The second limitation in GoldSim deals with the choice of distribution. Unless external input files to GoldSim include the capability to specify a distribution type for each input parameter, users will be limited to the distribution type specified within the GoldSim file. It is in theory possible to include a stochastic element for each distribution type that could be used for a selected uncertain variable, and include all of these possible choices in the GoldSim input file. However, in practical terms this would quickly become cumbersome as it would require thousands of GoldSim input elements. The LHS DLL removes this limitation.

The LHS DLL provides a tool that ensures reproducible results and allows the user more flexibility in selecting distributions to describe input data. The LHS DLL creates an input file, calls the LHS executable, reads the results, and exports them to GoldSim.

The DLL lhs_call is used to call the executable version of the LHS code (lhsdrv.exe) within GoldSim. All information relative to the sample properties and sampling strategy are defined in GoldSim elements and sent to the DLL. The DLL creates an input file (LHS_input.txt) for the executable, runs the executable, and reads the result file (LHS_OUTPUT.txt). It then sends the sample back to GoldSim in a 2D table in which each row represents a different realization and each column a different variable.

The distribution types that are available in the LHS DLL are shown in Table 4-4. A comparison between the DLL and GoldSim shows that GoldSim proposes 21 distributions offering some not available in LHS (e.g., Pearson, Boolean, extreme probability, and extreme value) and lacking others (e.g., geometric, hypergeometric, and maximum entropy). However, both the DLL and GoldSim include the most commonly used distributions.

The description of variable distributions and correlations can be put in arrays in GoldSim with each array becoming an input of the DLL. The DLL uses this information to generate an input that is read by the executable LHS code (lhsdrv.exe). The executable generates a sample that is then read by the DLL. The subsequent output is written in a format that can be read by GoldSim.

One of the design requirements for and benefits of using the DLL is to allow the user to choose different distributions for a selected input parameter. To this end, an MS Excel spreadsheet has been set up such that the user can use a drop-down menu to select (outside of GoldSim) a distribution for each variable. The user can specify the parameters related to each distribution (shown as P1 to P4 in Table 4-4) including the possibility of having a constant value (shown as P0 in Table 4-4). The MS Excel spreadsheet can be replaced with a more rigorous database (such as the external relational database under development and described in Section 4.2.2.2). It is possible to specify a value for P0 (deterministic) and values for P1 to P4 (uncertain) at the same time. The DLL will read only the appropriate information and ignore what is not necessary. For example, once the potential values are entered, the user can declare a constant value for an input variable for one simulation and then switch to a probability distribution for the same variable for the next simulation without having to re-enter any values. A correlation amongst variables can also be declared in MS Excel.

The DLL will be integrated into GPAM to support the sampling of uncertainty distributions given in the MS Excel input spreadsheet (Section 4.2.2.1). In the future, the DLL will also be used to support GPAM calculations after the implementation of the GDS Parameter Database (Section 4.2.2.2).

Given the early development stage, this software is considered QA-N/A. However, the QA status will be reviewed as development and application progress.

4.2.3 Configuration Management

As part of the UFD Campaign, the GDSM group has been assigned the task of conducting generic investigations of disposal options for UNF and HLW. To support these investigations, the group is developing (1) four GDS models, each for a different disposal environment, i.e., clay, granite, salt, and deep borehole, and (2) an integrated generic system-level model, i.e., the GPAM. This section discusses configuration management of three areas: parameters and the parameter values used in calculations, the four individual GDS models and GPAM, and calculations supporting the UFD Campaign.

4.2.3.1 Configuration Management Strategy

The plan for producing these models involved preliminary work on the individual GDS models and incorporation of these models into the system-level model. The plan for the individual GDS models involved working to two freeze points. The first freeze point was designed to provide the GPAM Lead modeler with preliminary versions of the individual models, which could be used to develop the preliminary version of GPAM. The second freeze point was designed to provide versions of the individual GDS models that were suitable for inclusion in the version of GPAM that will go forward. The second freeze point was April 29th 2011. Eventually the individual GDS models will be retired and all GDS calculations will be completed using the GPAM.

A configuration management policy has been developed to address configuration control on the parameters and the parameter values used in GDS calculations. The policy also addresses configuration management of the individual GDS models and GPAM. The policy has been implemented at the direction of the GDSM Manager.

Table 4-4. List of Available Distributions (and Associated Parameters) in LHS DLL

Dist. Number	Distribution Name	P0	P1	P2	P3	P4
1	normal		mean	stdev (>0)		
2	truncated normal		mean	stdev (>0)	lower q	upper q
3	bounded normal		mean	stdev (>0)	lower b	upper b
4	normal-B		value at q=0.001	value at q=0.999		
5	lognormal		mean (>0)	error fact (>0)		
6	lognormal-N		mean (>0)	stdev (>0)		
7	truncated lognormal		mean (>0)	error fact (>0)	lower q	upper q
8	truncated lognormal-N		mean (>0)	stdev (>0)	lower q	upper q
9	bounded lognormal		mean (>0)	error fact (>0)	lower b	upper b
10	bounded lognormal-N		mean (>0)	stdev (>0)	lower b	upper b
11	lognormal-B		value at q=0.001	value at q=0.999		
12	uniform		min	max (>min)		
13	loguniform		min (>0)	max (>0)		
14	exponential		lambda(>0)			
15	maximum entropy		min (>=0)	mu (>0)	max (>0)	
16	weibull		alpha (>0)	beta (>0)		
17	pareto		alpha(>2.0)	vbeta (>0)		
18	gamma		alpha	beta		
19	beta		min (>=0)	max (>0)	p (>0.001)	q (>0.001)
20	inverse gaussian		mu (>0)	lambda(>0)		
21	triangular		Min	mode (>min)	max (>mode)	
22	poisson		lambda(>0)			
23	binomial		p (0<p<1)	n (>1)		
24	negative binomial		p (0<p<1)	n (>1)		
25	geometric		p (0<p<1)			
26	hypergeometric		Nn	N1 (<Nr)	Nr (<Nn)	
100	constant	value				

The goals of the configuration management policy are:

- Maintain configuration control of parameters and parameter values
- Maintain configuration control of models
- Document calculations performed using the models
- Ensure reproducible results
- Establish management controls (GDS Run List)
- Coordination with process modelers

The GDSM Site on SharePoint®—The GDSM site on SharePoint is a central feature of this configuration management process. The site contains a library entitled "Configuration Management" to be used to support the actions discussed in this policy statement. The Configuration Management library is organized into the following folders: "Calculations", "Models", "Parameters", and "Templates and Examples". The Configuration Management Lead is responsible for maintaining the Configuration Management library. As such, he will work with modelers and others as needed to help ensure the appropriate files regarding parameters, models, and calculations are posted to the GDSM site. In the future the GDS Parameter Database will be hosted on an IT SharePoint site that is devoted to GDSM work.

Parameters—Eventually there will be a GDS Parameter Database, which will provide configuration control for parameters and parameter values used in GPAM. The parameters that are defined in the GPAM GoldSim Model file will determine the parameters in the database. However, there will not be a one to one correlation. The structure of the GPAM precludes this correlation. The model is divided into four domains, i.e., source, near field, far field, and biosphere. Parameters are defined in GPAM for these domains. However, calculations are performed for individual disposal environments, i.e., clay, granite, salt or deep borehole. Consequently, the database will need to have multiple potential values for a parameter such as far-field porosity. The multiple potential values will be required if the individual disposal environments use different values for the parameter. Additional values may be included in the database to support sensitivity analyses. Version control will be maintained for parameters and parameter values through a set of user levels with appropriate privileges.

The information in the GDS Parameter Database will be accessible through the SharePoint interface to the database. The information will be viewable on a series of forms that can be seen by all users. The definition of user levels will facilitate configuration management of the parameter information. Only people with User Level 1 designation will be able to enter or change parameter information in the database. People with User Level 2 designation will be able to review the parameter information in the database, provide comments, and indicate approval of the information, if appropriate. People with User Level 3 designation will have read only access to the database.

All information will be entered into the database initially by someone with User Level 1 designation. All subsequent changes to the information will be tracked within the database. When a new parameter is added to the database the status of the parameter is set to pending. Information about the parameter, as discussed in Section 4.2.2.2, is added to the database through a series of forms and drop down lists.

The information will be verified by an independent reviewer, who has Level 2 user status. When parameter information is initially input into the database the parameter status is identified as pending. After the parameter information is verified by the independent reviewer, the parameter status is changed to verified. The reviewer will evaluate the information for completeness and accuracy.

The baseline suite of parameters and parameter values will be maintained on this database. The identification of a "baseline" for the GDS Parameter Database may be a little different from what many people are used to. Typically a parameter baseline consists of a single value, or stochastic representation, for each parameter in a model. In the case of GPAM, this treatment is not possible.

The GPAM is designed to perform calculations for a variety of disposal environments. The variations to be investigated include different host rocks, i.e. clay, granite, and salt. The variations also include different disposal configurations, i.e. the deep borehole concept, as well as a variety of waste form types. Generic parameters have been defined in the GPAM to facility these calculations. These generic parameters may have different baseline values depending on the type of calculation, i.e. clay, granite, salt, or deep borehole concept. For instance, near-field porosity will have a different baseline value depending on whether the calculation is using clay, granite, or salt in the near field.

The generic nature of the calculations adds an additional complexity to the problem of baseline definition. There may be several values for a parameter that have been determined to be appropriate for the parameter in different granite environments, for instance. In this case the modeler has two options. The modeler, in conjunction with the subject matter expert if available, may decide that it is too early to define a baseline value for this parameter and the baseline value will be tracked as "to be determined" (TBD). Alternatively, the modeler, in conjunction with the subject matter expert if available, may compile all available information for the value of the parameter and develop an uncertainty distribution that incorporates all of the information. This uncertainty distribution will be used as the baseline value for the parameter. If either of these options is used the modeler needs to document it in the description section of the appropriate parameter list. It is also possible that some information will be tracked as TBD because of the preliminary nature of the information.

It is also likely that parameter information will be included in the database that is intended for use in sensitivity analyses. These input data values will be identified in the database as variants. It is possible that these variations may be included in uncertainty distributions for baseline parameter values. But the identification as "variants" indicates that these particular values are to be used in sensitivity analyses and are not to be considered part of the technical baseline.

These complexities make the identification and documentation of specific inputs for specific calculations even more important than it might be in other cases. The GDS Parameter database will have the capability of maintaining a record of the specific suite of parameters that are used for each individual calculation. In addition, the GDSM team will maintain documentation of individual calculations (discussed in more detail below).

Eventually the baseline parameter values will be coordinated with subject matter experts to ensure that the best available information is used for the baseline values. Justification of the baseline values will rest with these subject matter experts. However, at this early stage of the project subject matter experts may not be available to support this function. Until they are available, the modelers must provide an explanation for the parameter values used in the calculations.

Models—GPAM has been constructed using inputs from models developed for each of the four disposal environments. The evolution of GPAM will include inputs from a team of modelers. In this environment maintaining version control will be essential. The Configuration Management Library on the GDSM SharePoint site will be used to store the baseline version of GPAM. Version control will be maintained using the capabilities within GoldSim. Superseded versions of GPAM will be archived on SharePoint.

Calculations—As part of the configuration management strategy, the calculations made with the GDS models will be documented. In particular, documentation will be needed for calculations that are reported in a publication. Documentation will also be needed for calculations completed to test or evaluate a particular model. Examples include validation calculations and sensitivity analyses. The documentation will ensure that information is available to reproduce the calculation, if needed. The documentation will also help future workers who may want to use existing calculations as a starting point for developing new analyses.

A documentation package will be developed for each calculation that is done with one of the four individual GDS models or GPAM. This package will contain the GoldSim® model file, a copy of the parameter list from the GDS Parameter Database, and a GDS Analysis Description. The GDS Analysis Description will include the following: (1) identification of the purpose of the calculation, (2) a description of the calculation, (3) identification of changes to baseline parameter values, and (4) a description of the uncertainty characterization. The completed calculation documentation package will be stored in the Configuration Management Library on the GDSM site.

A template for the GDS Analysis Description is available in the Configuration Management library on the GDSM site. The library also contains two examples of a GDS Analysis Description: a short form appropriate for when the primary documentation of the calculation is in a publication that can be referenced, and a long form appropriate for when the GDS Analysis Description is the primary documentation. The individual modelers or any others producing calculations are responsible for generating the documentation packages and, in conjunction with the Configuration Management Lead as needed, posting the packages to the GDSM site.

The GDS Run List has been established as a management tool that will be used to track calculations planned for the GDSM group. This list will identify proposed calculations to be completed by each of the individual GDS models and by the GPAM. Other information on the list will be (1) the purpose of the calculation, (2) the anticipated, or actual completion date for the calculation, and (3) the location on SharePoint where documentation of the calculation can be found. The GDS Run List will be maintained by the Configuration Management Lead, but the content will be determined by the individual modelers or any others producing calculations.

4.2.3.2 Interim Approach

During the development of the GDS Parameter Database, interim tools have been developed to maintain configuration control. These interim tools have been developed using MS Excel and SharePoint. MS Excel spreadsheets have been used to document parameters and parameter values (Section 4.2.2.1). SharePoint has been used to store versions of the models and the parameter lists. Eventually these interim tools will be retired. There are two reasons that will lead to the retirement. The first is that the GDS Parameter Database will take over most of the functions being performed by the interim tools. The second reason is that the individual GDS models will be retired themselves, and be replaced by GPAM.

Parameters—The GDS Parameter Database is currently under development and will be for some time. In the interim, configuration control will be maintained using parameter lists in a spreadsheet format. Parameter lists are available for the Freeze Point 2 versions of the four individual GDS models on the GDSM site on SharePoint. An MS Excel-based input file is also being used for the GPAM until the GDS Parameter Database is operational. These parameter lists provide a tool for establishing a baseline, in the absence of a relational database. While the Configuration Management Lead is responsible for maintaining the parameter lists on the GDSM site, the content is ultimately the responsibility of the model developers.

The parameter lists were developed for each of the individual GDS models. The lists were developed by manually extracting information on individual parameters from the models and recording them in MS Excel files. The initial lists were developed from the Freeze Point 1 versions of the models. Subsequently the lists were updated to be consistent with the Freeze Point 2 versions of the models. The parameter lists were developed by the Configuration Management Lead and were subsequently reviewed and approved by the individual GDS model leads.

The parameter lists identify the GoldSim parameter name, as used in the model. For each parameter name the list provides information on the representation type, i. e. discrete or stochastic. If the parameter is included in the model as a stochastic then the parameter list identifies the type of stochastic used. The parameter list provides the value of the parameter that is used in the Freeze Point 2 version of the individual GDS model. The list also provides any descriptive information about the parameter that is included in the GoldSim model file and any additional comments that the model lead wants to include. The list also includes traceability information to help anyone using the list find the parameter in the GoldSim Model file.

The parameter lists for the Freeze Point 2 versions of the models define the baseline for the individual GDS models. Changes to this initial parameter information, due to error correction or evaluation of new information, will be documented in revisions to the parameter lists. The revised parameter lists will be stored on SharePoint. It will be important to use the parameter lists as documentation of inputs for individual calculations. A copy of the parameter list, with changes from the Freeze Point 2 version noted, will need to be part of the documentation of individual calculations (discussed in more detail below).

Models—The Freeze Point 2 versions of the four individual GDS models provide a partial baseline for the GDS numerical models. The version of GPAM that incorporates these Freeze Point 2 GDS models completes the initial GDS model baseline. Version control of these models must be maintained as the GDSM efforts move forward. The Configuration Management Library on the GDSM SharePoint site will be used to store the baseline versions of the models. The individual model developers will be responsible for maintaining the most current version of their model on the GDSM site. A standard versioning convention will be used with the models: Version x.yz. Use of this convention will begin with the Freeze Point 2 models. The initial version of the GPAM is also being stored on the GDSM SharePoint site. The GPAM is still under development, but versioning will be maintained as the development continues.

Calculations—As part of the configuration management strategy, the calculations made with the GDS models during the interim period will be documented. In particular, documentation will be needed for calculations that are reported in a publication. Documentation will also be needed for calculations completed to test or evaluate a particular model. Examples include validation calculations and sensitivity analyses.

The documentation package will be developed for each calculation that is done with one of the four individual GDS models or GPAM. This package will contain the GoldSim® model file, a copy of the parameter list developed for the model, and a GDS Analysis Description. The GDS Analysis Description will include the following: (1) identification of the purpose of the calculation, (2) a description of the calculation, (3) identification of changes to baseline parameter values, and (4) a description of the uncertainty characterization. The completed calculation documentation package will be stored in the Configuration Management Library on the GDSM site.

4.3 Incorporation of Individual GDS Models into GPAM

The GPAM provides a common conceptual framework to enable evaluations and comparisons of disposal system alternatives. The four individual GDS models (granite, clay, salt, and deep borehole) described in Section 3 will be implemented within the GPAM framework. This will allow for more consistent evaluations and comparisons of the various UFD disposal system alternatives. Table 4-5 provides a mapping that correlates the Freeze Point 2 model domains of each individual model to the common GPAM domains.

Once the individual GDS models have been implemented within the GPAM framework, each of the four GPAM representations will need to be (1) tested/validated against the corresponding individual model, and (2) validated against relevant PA results from other radioactive waste disposal programs.

Table 4-5. Individual GDS Model Components Correlated to GPAM Model Domains

GPAM Domain	Salt GDS Model[a]	Granite GDS Model[b]	Clay GDS Model[c]	Deep Borehole GDS Model[d]
System Level – Repository Configuration	\Near_field \NearField_Config \Salt_NF_volume	\Container1 \near_field_new \Repository_config \GDSE_NF_volume	\Parameters and Material	\Deep_Borehole_Data
System Level – Radionuclide Species	\Materials • Species	\Materials • Species	\EBS_and_NearField \EBS Properties • Species	\Materials • Species
System Level – Inventory	\RN_Inventory \UNF Inventory • UNF_Total_isotope_mass *[parallel structure for DHLW and CHLW inventory not shown]*	\Container1 \RN_Inventory \UNF_Inventory • UNF_Total_isotope_mass *[parallel structure for DHLW and CHLW inventory not shown]*	\EBS_and_NearField \EBS Properties • Total_ Isotopic_ Mass	\RN_Inventory \UNF Inventory • UNF_Total_isotope_mass *[parallel structure for DHLW and CHLW inventory not shown]*
System Level – Temperature	\Near_field \NearField_Config \WP_thermal • WP_temp	\Container1 \near_field_new \Repository_config \WP_thermal • WP_temp	Not specified	\Deep_Borehole_Data \WP_thermal • Canister_temp
System Level – Reference Fluid Properties	\Materials • Water	\Materials • Water	\EBS_and_NearField \EBS Transport \Degraded_Waste_Form • Water	\Materials • Water
System Level – Property Libraries	N/A	N/A	N/A	N/A

Table 4-5. Individual GDS Model Components Correlated to GPAM Model Domains (continued)

GPAM Domain	Salt GDS Model[a]	Granite GDS Model[b]	Clay GDS Model[c]	Deep Borehole GDS Model[d]
Source Term – Waste Form	\Near_field \Waste_form_degradation • SOURCE = UNF_Release \Near_field \Waste_form_degradation \UNF_Release • 1 CELL - Cell1_UNF_WF • FLUID = Water • SOLID = N/A *[parallel structure for DHLW and CHLW source terms not shown]*	\Container1 \near_field_new \Waste_form_degradation \UNF_WF • SOURCE = UNF_1diffWP _release \Container1 \near_field_new \Waste_form_degradation \UNF_WF \UNF_1diffWP_release • 1 CELL - Zone1_Z4R1_U • FLUID = Water • SOLID = Waste *[parallel structure for DHLW and CHLW source terms not shown]*	\EBS_and_NearField • SOURCE = EBS_Transport \EBS_and_NearField \EBS Transport \Degraded_Waste_Form • 1 CELL - Degraded_Waste_Form_ C • FLUID = Water • SOLID = WF_Debris	\DBH_RN_release \DBH_WF_release • SOURCE = DBH_ UNF_ Inventory_Case1 \DBH_RN_release \DBH_WF_release \DBH_UNF_Inventory_Case1 • 1 CELL - Cell1_DBH_UNF_Case1 • FLUID = Water • SOLID = N/A *[parallel structure for DHLW and CHLW source terms not shown]*
Source Term – Waste Package	\Near_field \WF_RN_release • Total_WF_Release *[Collects mass from commercial UNF, DHLW, and CHLW source terms]*	\Container1 \near_field_new \Waste_form_degradation \UNF_WF \UNF_1diffWP_release • 27 CELLS (2D: 4x8, less 1) - Zone2_Z#R#_U • FLUID = Water • SOLID = Bentonite *[parallel structure for DHLW and CHLW source terms not shown]*	\EBS_and_NearField \EBS Transport \Degraded_Waste_Package • 1 CELL - Degraded_Waste_ Package_C • FLUID = Water • SOLID = WP_Debris	\DBH_RN_transport \DBH_Transport_DisposalZone \DisposalZone_MultipleCells \DisposalZone_Transport \DZ_LongSeg_Property • WFRelease_Case1_LongSeg \DZ_ShortSeg_Property • WFRelease_Case1_ShortSeg *[Collects mass from commercial UNF, DHLW, and CHLW source terms]*

Table 4-5. Individual GDS Model Components Correlated to GPAM Model Domains (continued)

GPAM Domain	Salt GDS Model[a]	Granite GDS Model[b]	Clay GDS Model[c]	Deep Borehole GDS Model[d]
Near Field – EBS Inner	\Near_field \WF_RN_release \NF_MixingCells • 5 CELLS - NFMixingCell_# • FLUID = Water • SOLID = RepBlock_Salt _Medium	\Container1 \near_field_new \WF_RN_release \WF_RN_Release_Case1 • 1 CELL - Diff_NF_Mixing_Cell _Case1 • FLUID = Water • SOLID = N/A *[Diff_NF_Mixing_Cell collects mass from commercial UNF, DHLW, and CHLW source terms]*	\EBS_and_NearField \EBS Transport \Secondary_EBS • 3 CELLS (Matrix) - Secondary_EBS_# • 3 CELLS (Fracture) - Secondary_EBS_#F • FLUID = Water • SOLID = Secondary_EBS_ Medium	\DBH_RN_transport \DBH_Transport_DisposalZone \DisposalZone_MultipleCells \DisposalZone_Transport \DisposalZone_5000_4000 • 50 CELLS (LongSeg Cells) \DisposalZone_4000_3000 • 50 CELLS (ShortSeg Cells) • FLUID = Water SOLID = Medium_Disposal _Zone
Near Field – EBS Outer	\NF_Interface \IF_SaltBlock_Transport \IF_MixingCells • 5 CELLS - IFMixingCell_# • FLUID = Water • SOLID = IF_Salt_Medium	\Container1 \NF_Interface • 1 CELL - Near_to_far_field _collector • FLUID = Water • SOLID = N/A	\EBS_and_NearField \EBS Transport \Excavation_Damage_Zone • 3 CELLS (Matrix) - EDZ_# • 3 CELLS (Fracture) - EDZ_#F • FLUID = Water • SOLID = EDZ_Medium	\DBH_RN_transport \DBH_Transport_SealZone \SealZone_MultipleCells \SealZone_Transport \SealZone_3000_2000 • 50 CELLS • FLUID = Water • SOLID = Bentonite_Seal_ Zone
Near Field – Host Rock	\NF_MB_Transport \NF_MB_Transport \NFMB_MixingCells • 5 CELLS - NFMB_MixingCell_# • FLUID = Water • SOLID = Salt_NFMB _medium	N/A	N/A	N/A

Table 4-5. Individual GDS Model Components Correlated to GPAM Model Domains (continued)

GPAM Domain	Salt GDS Model[a]	Granite GDS Model[b]	Clay GDS Model[c]	Deep Borehole GDS Model[d]
Far Field – Host Rock	\FF_MB_Transport \FFMB_MixingCells • 5 CELLS - FFMB_MixingCell_# • FLUID = Water • SOLID = Salt_FFMB_medium	\Container1 \Far_Field \FEHM_localize • 1 DLL - ExternalPathway_fehm • FLUID = N/A • SOLID = N/A	\Far_Field \Clay_Far_Field_Cells • 400 CELLS (2D: 20x20) - Zone1_X##Y## • FLUID = Water • SOLIDS = Clay, Clay_X, Clay_Y	N/A
Far Field - Aquifer	\FF_MB_Transport • 1 CELL - Far_field_sink	\Container1 \Far_Field \sink • 1 CELL - Far_field_sink	\Aquifer • 1 CELL - Aquifer_Cell	\DBH_RN_transport \DBH_Transport_UpperZone \UpperBHZone_Pipe • 1 PIPE - UpperZone_Pipe • 1 CELL - UpperZone_sink • FLUID = Water • SOLID= Seal_UpperBH
Biosphere - Receptor	\Results • 1 RECEPTOR - Dose_Rate_ERB1B	\Container1 \Results • 1 RECEPTOR - Dose_Rate_ERB1B	\Biosphere • 1 RECEPTOR - Calculate_Dose_Rate	\DBH_Results \Dose_MultiplePipes • 1 RECEPTOR - DBH_DoseResults_Case1_MultiplP
Fast Path	\Brine Pocket Flow [in file *GDSE Salt FY11 Baseline v2 (HI Scenario May09-2011).gsm*][e]	\Container1 \Human Intrusion [in file *generic_granite_disturbed_36species+Dummy_FY11report.gsm*][e]	\Fast_Path_Scenario	N/A

NOTE: [a] Based on Freeze Point 2 model file *GDSE Salt FY11 Baseline v2 (Ref Scenario May09-2011).gsm*
[b] Based on Freeze Point 2 model file *generic_granite_undisturbed_36species+Dummy_FY11report.gsm*
[c] Based on Freeze Point 2 model file *FY11_Clay_GDSE_Model_0104.gsm*
[d] Based on Freeze Point 2 model file *DBH FY11(Baseline v2_Apr29-2011).gsm*
[e] Implementation of Fast Path capabilities requires a separate file

4.4 GPAM Future Versions

The modular architecture of the GPAM conceptual framework makes it easy to revise and/or upgrade specific GPAM regions and/or model domains. GPAM V0 is an initial version to demonstrate the implementation of a common framework and linkages to external input files. Future versions will have added capabilities to better represent all potentially relevant FEPs. Many desired future capabilities were identified in Sections 4.1 and 4.2. They are summarized here.

- System-Level
  - Specify simulation settings within MS Excel (Section 4.2 and 4.2.2)
  - Specify radionuclide species, chains, half-lives, atomic weights within MS Excel (Table 4-3 and Section 4.2.2)
  - Add the capability to externally select input value distributions, with the LHS DLL or a built-in GoldSim functionality (Section 4.2.2.3)
  - Consolidate worksheets in the MS Excel input file to have a more direct one-to-one correspondence with the GoldSim model domain input containers (Section 4.2.2.2).
  - Add the capability for model domains to be unsaturated (fluid saturations less than 1) (Section 4)
  - Add the capability for explicit temporal and spatial specification of temperature, and the corresponding dependence of other parameter values on temperature (Table 4-3 and Section 4.2.1.1).
  - Add the capability for time-varying parameter values (Table 4-3).
  - Variable number of elements in each model domain, variable transport length of each element within a model domain (Section 4.2.1)
  - Add the capability to de-activate or bypass model domains (Section 4.2.1)
  - Create GoldSim Result elements within the GPAM model file and implement the capability to export the results to external files (Sections 4.2 and 4.2.1.11)
  - Explore the capability to simulate multiple GPAM transport pathways with different inventories and/or characteristics (Section 4.2.1.1).
- Source Region
  - Add an instant release fraction from waste form (Section 4.2.2)
  - Add the capability for a user-specified combination of inventories (Section 4.2.2)
  - Add the capability to represent colloidal formation and transport (Section 4.2.1.2)
  - Add the capability for a multi-cell source region, such as is required for the Deep Borehole concept (Section 3.4.1.3)
- Near-Field and Far-Field Regions
  - Incorporate more complex Source and Near Field (EBS) model domains and/or components, as appropriate (Section 5)
  - Make the Near-Field and Far-Field Host Rock 2D transport cells functional (Table 4-3 and Section 4.2.1.6)
  - Add the capability to use the FEHM DLL (Section 3.2.2.6)
  - Add the capability for matrix diffusion in the Near-Field and Far-Field Host Rock. The capability may be added by (1) parallel dual porosity cells as in the EBS, (2) input of GoldSim matrix diffusion parameters for Pipes, or (3) using the FEHM DLL (Table 4-3 and Section 4.2.1.6).
  - Examine whether a new GoldSim transport element, called an Aquifer, can be used to replace some of the existing pipes and cells and/or eliminate the need to “select” between a pipe (advective) pathway and a cell (diffusive) pathway in certain model domains (Section 4.2.1).
- Fast Path
  - Add the Fast Path capability (Sections 4.2.1 and 4.2.1.10)

5. EBS MODEL ARCHITECTURE DEVELOPMENT

5.1 Introduction

In order to further develop GPAM with the needed flexibility, a re-examination of the treatment of the natural system and EBS will be done. This re-examination will establish a common and comprehensive structure to address the FEPS associated with disposal options and to implement these FEPs at appropriate levels of detail for various applications. The natural system restructuring will occur in FY 2012. The evaluation and restructure of the EBS began in FY 2011, and implementation into the GPAM is planned for FY 2012.

System engineering principles will be applied to the development of successively more detailed versions of GPAM in FY 2012 and beyond. The approach is intended to apply lessons learned from previous PA efforts (Yucca Mountain, WIPP) to enable GPAM such that it is calculationally efficient and transparent to explain. Control of model and software requirements during development will help ensure that the model is efficient, and that results for different media, waste streams, etc. can be compared in ways that are meaningful to stakeholders in waste management decision-making. Description of GPAM using a common architecture emphasizes the essential similarity of the different disposal options, while providing a framework and nomenclature for discussing their differences. Early definition and control of GPAM model architecture will facilitate site-specific model development and FEP analysis.

The starting point for this discussion is the FY 2011 GPAM V0 description (Section 4). The architecture for GPAM V0 is relatively simple (compared to previously published PA models such as Yucca Mountain), but is robust and flexible. This section is a general roadmap for elaboration of the GDSM effort to include additional FEPs, particularly disruptive events, and to accommodate more detailed simulation approaches.

5.2 Lessons Learned from Yucca Mountain and WIPP PA Models

The following lessons learned were distilled mainly from comparison of the PA models for the Yucca Mountain Total System Performance Assessment (TSPA) and WIPP PA. The Yucca Mountain TSPA described a more complex disposal concept, and could have benefitted from some of the lessons learned from the WIPP PA.

- *Lesson Learned #1*—Make model architecture as transparent as practical.

  This will be accomplished by (1) using a common system architecture for disposition of FEPs prior to PA model build, and (2) associating included and excluded FEPs with potentially affected architecture elements and interface conditions. A simple, modular architecture facilitates "insight" studies that prioritize key model components (i.e., FEPs) that affect safety. It also facilitates model documentation and verification/validation, isolation of barriers or sub-scenarios for study, and FEP screening.

- *Lesson Learned #2*—Simplify model architecture.

  Realistic models for disposal concepts such as that proposed for Yucca Mountain tend to be challenging to explain due to the complexity of numerous model components and their interconnections, particularly if the representation becomes highly abstracted. As this complexity evolves during development of generic or site-specific models, change control processes will be used to control technical review and resource demands on the developers.

- *Lesson Learned #3*—Limit the number of distinct models and software tools with similar functions.

  Redundancy tends to compromise consistency and makes it more difficult to check the work of others (without specialized knowledge). Software tools should be flexible (e.g., programmable) and universally available in a structured, integrated computing environment.

- *Lesson Learned #4*—Limit the use of abstraction.

  As alluded to above, use of abstraction tends to reduce transparency, particularly for complex systems. Pre-calculating subsystem responses for a limited number of uncertainty vectors (e.g., lookup tables, breakthrough curves) limits the system model utility. Also, neglecting the co-dependence of other subsystems requires additional justification. To the extent possible, numerical simulations should be initiated and performed within the system model, incorporating more fundamental descriptions of science The WIPP PA tended toward this direction. As an alternative to abstraction, alternative (i.e., simplified) algorithms can be developed to emulate underlying process models, and implemented directly within the system model. The advantages of this approach are described in a recent international summary (Bailey et al. 2011):

  > *Simple analytic expressions or very simple models can be useful for communication purposes and build confidence in the results of the complex numerical models, by showing that similar results are obtained using simple models whose basis may be more easily explained and that can be shown to capture the essential features of the system. This agreement between simple and complex models would demonstrate a good understanding of the repository behaviour and that the key processes and parameters have been identified.*

- *Lesson Learned #5*—Make model complexity commensurate with importance and intended application.

  This can be accomplished by: (1) provide modularity so that simpler (or more complex) calculations can be substituted for debugging and sensitivity analysis; (2) design the modules to include or exclude FEPs based on *a priori* reasoned approaches and not resource availability; and (3) choose modules or modeling approaches to be commensurate with the relative importance of the model to system performance.

- *Lesson Learned #6*—Elicit process modeling input to PA model development.

  Communication between PA analysts and the developers for underlying models will need to be maximized in order to implement the lessons described here. Barriers to communication such as geography and schedule will be managed so that process modelers fully understand and support the technical adequacy of the PA model. This will be accomplished by: (1) assimilating modelers into the PA development team; (2) using simulation instead of abstraction (see above); and (3) configuration management (see below). Cross pollination of PA and subject matter experts is critical to success.

5.3 EBS and System Architectures

A simple, effective system architecture is presented for the generic PA model in Section 4 (Figure 4-1). This section adds elements to that architecture, especially for the EBS, to represent design options and possible degraded states. It also describes the interfaces between elements, as context for a discussion of disruptive events, and later discussion of model requirements.

The term "system architecture" as used here is represented by a diagram of connected elements, each representing a subdomain of the disposal system, including both engineered and natural features. The EBS and natural barriers are separate domains, and the elements comprising those are arranged in subdomains (e.g., waste form, waste package, etc.). As presented (Figure 5-1) the EBS portion of the architecture includes one waste package and its contents, plus the other elements of the EBS at that location, and the backfill, seals, and plugs along potential transport pathways from that location. Other waste package locations may contribute radionuclide fluxes along the transport pathway, which may be important if they affect flow processes and/or radionuclide attenuation. Whereas the repository will contain many thousands of waste packages, this picture is repeated for many waste package locations (scaling can be used to represent sets of waste packages at such locations, where spatial uncertainty is understood). In the system model, the replicates are connected at far field, upstream and downstream interfaces where the physical and chemical conditions important to PA (or model accuracy) are not significantly affected by contributions associated with individual waste package locations (e.g., can be described as constant). The system architecture will be defined to facilitate this replication concept.

The primary focus of this discussion is the EBS architecture, which is likely to be more complex than the natural system. However, the overall system must be considered because the EBS influences the entire system (e.g., heat and released radionuclides), and because calculation of conditions within the EBS may require far-field boundary conditions that encompass the natural system. In other words, the EBS architecture can only be implemented successfully when the natural system is considered; hence a system architecture approach is needed.

A proposed system architecture for a generic disposal environment for UNF and HLW is shown in Figure 5-1. The diagram shows possible additional EBS features or subdomains (relative to Figure 4-1) that will be implemented in future GPAM development. Features or subdomains can be added, or deleted from this conceptual diagram as appropriate. Some important aspects of this approach are as follows:

- Implementation of engineered and natural barrier features in the GPAM can be 1D, 2D or 3D, as appropriate for model applications, although the diagram is essentially for 1D.
- Diagram elements can be deleted by using by-passing if these features are not included in the disposal concept, or if short-circuited in a disruptive scenario.
- Elements can change with simulation time, modified by internally driven (e.g., heating, corrosion) or externally driven (e.g., climate change, erosion) processes, or disruptive events.
- The system architecture diagram (Figure 5-1) represents radionuclide transport. Representing the movement of groundwater or other carrier fluxes, particularly upstream of the waste form, may require additional features.

The EBS architecture is based on a single waste package, which may contain an insert or filler material, and may have corrosion allowance or corrosion resistant elements for containment, as well as structural elements (Figure 5-1). The waste package may be surrounded by a reservoir (McKinley et al. 2006), and may be supported by a pedestal. Clay buffer and radionuclide getter materials may surround the waste package, and these may be enclosed in a prefabricated envelope to facilitate handling and emplacement. Getters are placed to sorb or precipitate selected radionuclides. If waste packages are emplaced in boreholes, seals and/or plugs may be used to control the mechanical or hydrologic responses, or for shielding. The far-field EBS includes backfill in emplacement drifts and access drifts, and may also include emplacement of low level waste or greater-than-class-C waste. Beyond the backfill, radionuclides may migrate within the EDZ, and plugs and seals would likely be used to control this pathway in the far field. Such an engineered system, together with natural barriers, is expected to provide a robust barrier to radionuclide migration to the accessible environment.

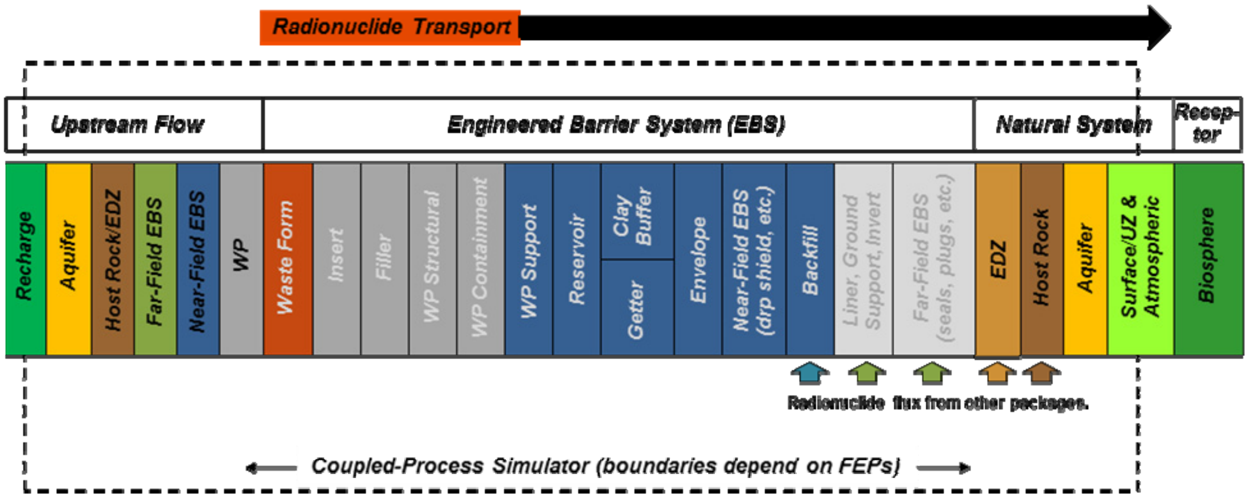


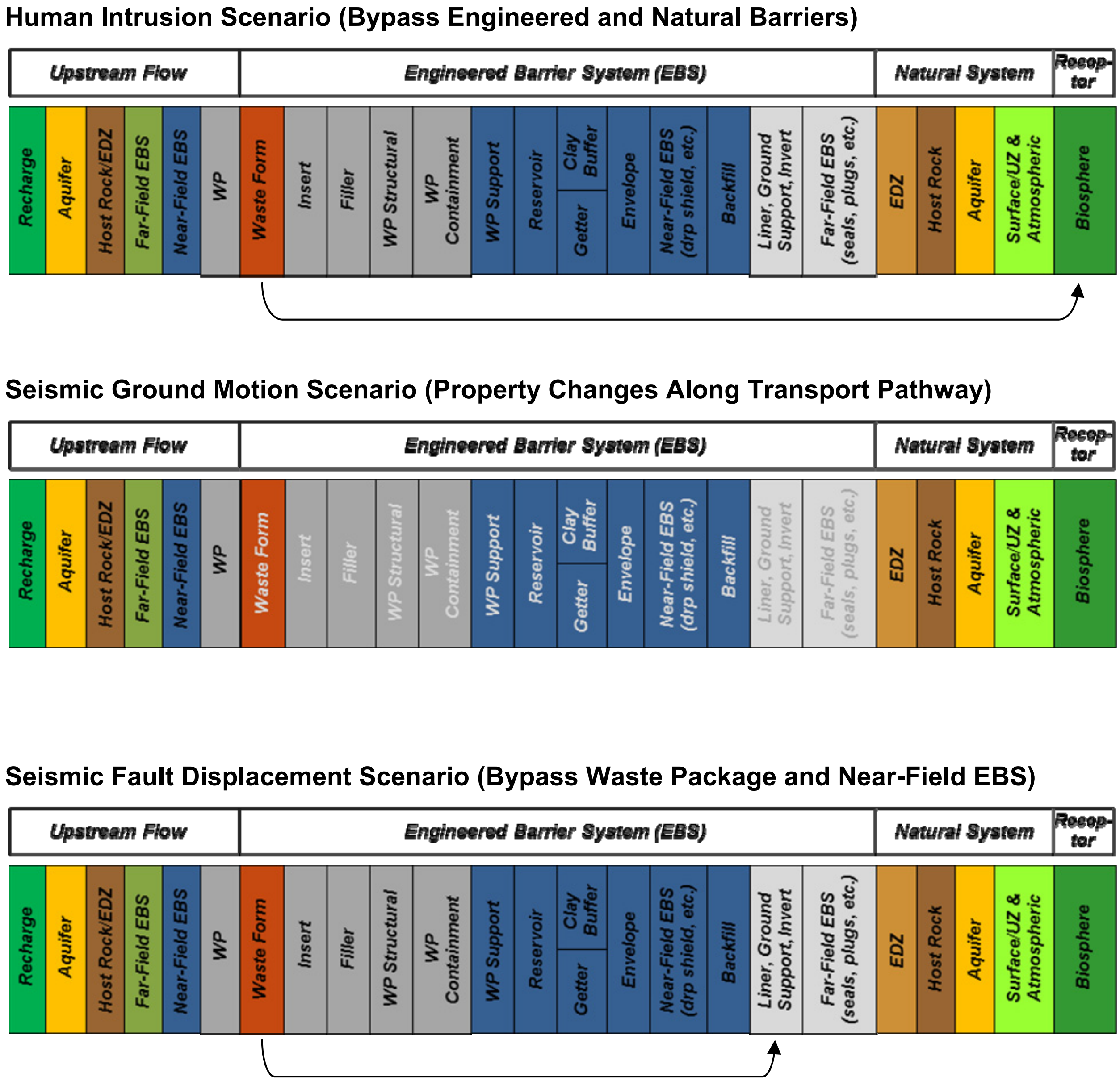
Figure 5-1. System Architecture Proposed for Future Model Development

5.3.1 Interfaces

Interfaces between system architecture elements are where mass and energy fluxes, and potentials such as temperature or radionuclide concentration, are defined at adjoining domain or subdomain boundaries. Interfaces (and architecture elements) are defined using a rational numbering/naming convention. Modular model components correspond to domains or subdomains, respect their boundaries, and provide all required interface data.

Multi-physics simulations used in the system model may cross the domains or subdomains in the system architecture, but they will also respect the appropriate boundaries and provide interface data (see requirements discussion). In general, use of numerical simulation in the system model is expected to increase accuracy and decrease complexity at interfaces, while ensuring mass and energy balances (as implemented in the simulation). Redundant simulations will not be used, i.e., the same physics will not be calculated for the same subdomain(s) by different models, to avoid the necessity of explaining or defending different predicted behavior.

Disruptive events such as seismic ground motion, faulting and human intrusion change the system in various ways that are readily described using the system architecture. For example, human intrusion simply short-circuits the waste form to the biosphere (Figure 5-2). Note that radionuclide transport may still occur through the engineered and natural barriers. Seismic ground motion has the principal effect of changing the configuration and properties of the engineered barriers (Figure 5-2), considering that the natural barriers have been exposed to comparable ground motion many times in the geologic past. Fault displacement intersecting one or more waste packages will change the properties of the EBS locally, while redirecting radionuclide transport to the far field at these locations. This results in multiple simultaneous release pathways governed by different representations. These scenarios may involve increased water flow into the repository, which could require additional elements as discussed previously. All of these scenarios can be readily described using the system architecture being developed, particularly for analysis and screening of FEPs.



NOTE: The features with property changes along the transport pathway for the seismic ground motion scenario (middle diagram) are denoted by the white and gray text.

Figure 5-2. Scenario Development using EBS and System Architecture

5.4 Software

The software environment for GPAM will evolve to take advantage of developments in modern information technology and computational resources. The objective is to implement the PA methodology, which is 30 yr in development (Bonano et al. 2010), for an evolving waste program. The mission will require generic feasibility and comparative studies, sensitivity analyses, and eventually, site-specific assessments. The software environment will facilitate a large number of models and variations, with "push-button" capability to replicate or modify previous work. Such a capability was developed to implement the PA methodology at WIPP (Vaughn 2010) and the need has been recognized internationally (Griffault et al. 2011). Further development of the software environment will help to ensure success of the anticipated future mission of the UNF and HLW management program in the United States.

The highest level of control evident to a user of an enhanced software environment for PAs and the one utilized here is the "framework function" (Vaughn 2010). This function will provide a user interface and "threading" of various data files, model algorithms, numerical simulations, and post-processors, all within a controlled environment. The power of the user interface determines the extent of manual scripting required. Version control and data management functionality are included. Framework tools exist in other disciplines, for example, software development, and such tools might be adapted for use in a PA.

The next lower level of functionality in a PA software environment is model implementation. Tools such as GoldSim provide object-oriented code modules that can be combined to represent some or all of the disposal system architecture elements, in a graphical context. In this way, all or many features of the EBS and natural system can be readily represented using commercial off-the-shelf software. Available commercial software, including tools developed for dynamic programming, can accomplish many of the functions of a framework tool. The GPAM (Section 4) is implemented in this manner using GoldSim. However, as mission complexity increases, a more specialized framework tool will be needed. Part of the FY 2012 effort will be to conduct an evaluation of currently available framework tools against specified requirements. The evaluation will include recommendations for a path forward that progresses beyond the first stage of development and focuses on future DOE-NE needs.

Code modules for numerical simulation can be called from GoldSim and similar tools, hence for convenience they are assigned here to the next lower level of functionality in the PA software environment. In principle, such codes can implement any model features, and thereby accomplish the functions of GoldSim and similar tools. In practice, multiphysics simulation technology has not yet been developed to represent features and processes such as waste form and waste package degradation, or biosphere processes, or scenarios such as human intrusion. So for the next few years there are appropriate, separate roles for both model implementation tools and numerical simulators.

5.5 Requirements

The functional requirements for a PA software environment will be implemented in framework, model implementation, and simulation tools. This section proposes functional and nonfunctional requirements, as a starting point for future specifications.

Model Requirements—Disposal system models created in a PA software environment will respect the following:

- Quantify performance measures as defined and/or required by regulations.
- Based on analysis of included and excluded FEPs, performed using a system architecture that is a complete representation of all EBS and natural system elements, domains, subdomains, and interfaces.

- Preserve modularity of architecture elements and domain/subdomain models to the extent practical.
- Maintain relative complexity of model elements commensurate with influence on dose and intended use.
- Provide the flexibility to capture all anticipated disposal options while preserving the ability to model specific site-selected options with sufficient complexity. This requires the ability to swap appropriate science descriptions of FEPs into and out of the framework.
- Avoid redundant model components, i.e., disallow separate models that represent the same FEPs within the same subdomain(s), using different calculation approaches that produce different results.
- Describe the PA model using a consistent, controlled nomenclature for domains, subdomains, interfaces, fluxes, and potentials.
- The PA model and its components will implement mass and energy balances in a way that can be verified.

Software Requirements—Software tools will include or support the following:

- Probabilistic analysis, including LHS sampling
- Threading of external applications (e.g., use of .dll code modules)
- Testing and control of numerical accuracy
- Run-time intervention (i.e., save intermediate results for restart, branching, or debugging)
- Configuration management for algorithms, scripts, code modules, input/output data, and supporting documentation
- Data management
- Graphical user interface
- "Plug and play" environment

Nonfunctional Requirements—A PA software environment will implement other requirements that are not directly related to model functionality, such as:

- Integrated software environment
- Access control and security

Configuration management processes can be used to promote integration among technical staff working on process models, PA model implementation, and the software environment. Change control that involves written proposals, review, and deliberation by a control authority, is a proven mechanism to promote integration among technical specialists and among different organizations. Variants of change control were adopted by both the WIPP and Yucca Mountain projects at critical junctures, to preserve model fidelity and consistency in a resource-limited project execution environment.

6. CONCLUSIONS

The GDSM team is focused on developing the modeling capability needed to evaluate various generic disposal environments and waste form options such that it evolves with the maturing needs of the DOE-NE/UFD mission. Their efforts support the UFD Campaign and the broader FCT Program. The following summarizes the key GDSM accomplishments during FY 2011:

- Further developed the individual GDS models for salt (Section 3.1), granite (Section 3.2), clay (Section 3.3), and deep borehole (Section 3.4) disposal environments. This work was coordinated with the development of the initial GPAM architecture to facilitate the integration of the capabilities of the individual GDS models into the GPAM.
- Mapped the four individual GDS models in terms of the relevant UFD FEPs (Section 2 and Appendix B)
- Developed the initial GPAM architecture (Section 4)
  - Designed with the flexibility to evaluate different disposal environments as well as waste form options and to handle different levels of scientific detail and sophistication in a fashion that it supports and utilizes evolving science efficiently
  - Created an LHS DLL to work with the GPAM GoldSim model file (Section 4.2.2.3; Sallaberry 2011). The LHS DLL ensures reproducible results and allows the user more flexibility in selecting distributions to describe input data.
  - Worked on the initial design for the GDS Parameter Database, which will be a key part of the long-term configuration management strategy (Section 4.2.3). In the meantime, an interim strategy was established.
- Applied a systems engineering approach to learn from past PA efforts and to develop a more detailed description of the EBS and systems architecture for consideration in the future (Section 5)
- Conducted a process-level investigation of diffusion modeling in a clay repository (Appendix A). Data sets of parameters relevant to diffusive transport in clay were reviewed from literature and compiled. A review was completed of phenomenological approaches to model diffusive transport versus mechanistic approaches. An improved modeling approach was proposed to combine the advantages of both approaches.

The report identifies multiple areas that would benefit from continued investigation, development, and/or improvement. Various discussions in Section 3 identify opportunities for improving the modeling capability of the different generic disposal environments. Section 4.4 summarizes recommendations for improving the GPAM structure and functionality. Section 5 outlines an approach that permits a common architecture to represent EBS processes and environments at varying levels of scientific detail. The next steps in adding scientific complexity are also described. Some potential improvements or refinements are discussed in general terms that are common to all of the disposal environments, such as improving the treatment of coupled processes to better represent the time-dependent evolution of the EBS and near field, the degradation of EBS components, and the representation of potential waste streams and inventory estimates. Sometimes the discussion is more specific to the particular disposal environment, e.g., the closure and consolidation of salt rocks by creep deformation under the influence of thermal perturbation, and the effect on the engineered barrier and near-field performance (Section 3.1.5). Appendix A contains recommendations specific to improvements for diffusion modeling in a clay environment.

The planning for future GDSM goals and activities is taking into account the possible improvements described in this report in conjunction with the potential needs of the UFD Campaign and FCT Program. One outcome has been the establishment of the following one-year goal for GDSM (corresponding to FY 2012):

> *Have in place a first-iteration, flexible system architecture that includes a preliminary model interface to an external computational database. Utilize current information available from the natural system, EBS, and loading management and design subject matter experts. Demonstrate the capability of the system model to provide disposal risk information to UFD and Systems Engineering Campaign decision makers.*

To support this goal, FY 2012 activities will include refinement of the capability to model the individual disposal environments. Another activity will focus on the development of a far-field flow architecture that enables a common model implementation. The GPAM itself will continue to be developed along with the supporting GDS Parameter Database. It is important to note that the development of the initial GPAM architecture in FY 2011 marks the start of the transition away from the four individual GDS models and to the GPAM. This transition will continue into FY 2012. Once the transition to the GPAM is finished, future development of or improvement to the modeling capability for the different generic disposal environments will be made within the GPAM framework rather than the individual GDS models. Increased coordination with the natural system, EBS, and loading management and design subject matter experts is expected to facilitate use of the current information available from them. In addition, a systematic evaluation will be conducted to investigate capabilities of other potential framework tools. Another GDSM activity will be to develop a generic safety case for deep geologic disposal in a holistic and comprehensive fashion. This activity will allow PA, which is but one component of safety, to be appreciated within the larger context of the generic safety case.

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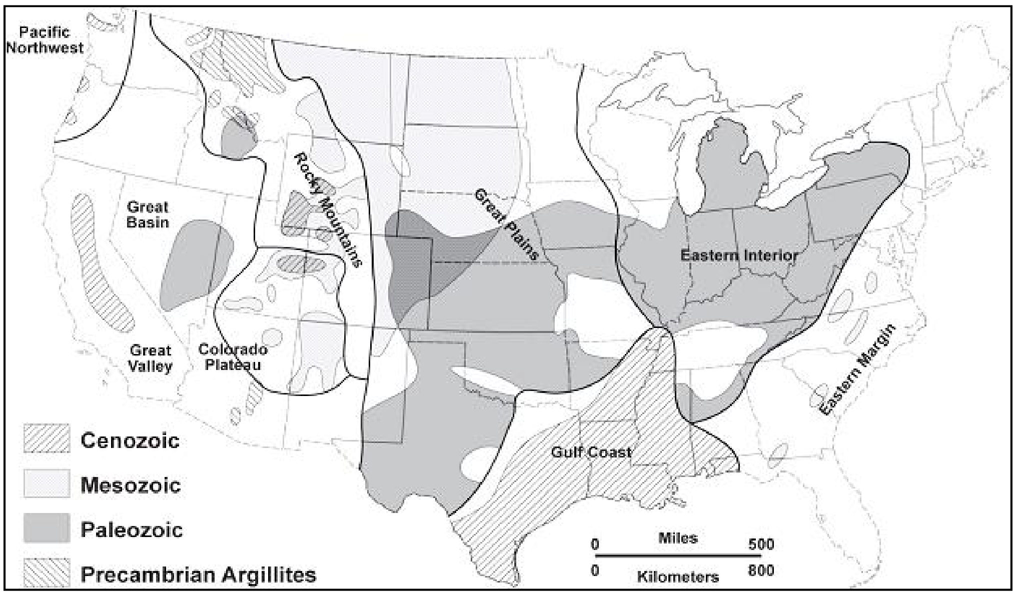
Appendix A

Diffusion Modeling in a Generic Clay Repository

A-1. Introduction

Clay/shale has been considered as potential host rock for geological disposal of UNF and HLW throughout the world, because of its low permeability, low diffusion coefficient, high retention capacity for radionuclides, and capability to self-seal fractures. For example, Callovo-Oxfordian (COx) argillites at the Bure site, France (Fouche et al. 2004), Toarcian argillites at the Tournemire site, France (Patriarche et al. 2004a), Opalinus Clay (OPA) at the Mont Terri site, Switzerland (Meier et al. 2000), and Boom clay at the Mol site, Belgium (Barnichon and Volckaert 2003) have all been under intensive scientific investigation (at both field and laboratory scales) for understanding a variety of rock properties and their relationships to flow and transport processes associated with geological disposal of radioactive waste. Figure A-1 presents the distribution of clay/shale formations within the USA.



Source: Gonzales and Johnson 1984.

Figure A-1. Clay/Shale-Formation Distribution in the USA

Owing to the low permeability of clay rock, diffusion may be the dominant mechanism for radionuclide transport in a clay formation. Exceptions possibly include areas where flow velocities may be larger, e.g., within the EDZ where highly-permeable fractures are induced by tunnel excavation or along natural features such as faults or intrusions disrupting the formation. The overall objectives of this work activity are to summarize the state of the art for modeling diffusion process in natural clay formations, to review analysis results from diffusion experiments on clay rock that are available in the literature, to evaluate the impact of relevant processes on diffusion, and to develop simplified diffusion process models that can be used to support the development of the system-level diffusion model for natural clay formations. This work activity addresses Features, Events and Processes FEP 2.2.09, Chemical Process—Transport (shale), which has been ranked medium in importance, as listed in Table A-7 of the *Used Fuel Disposition Campaign Disposal Research and Development Roadmap* (FCR&D-USED-2011-000065 REV 00) (Nutt 2011).

This report documents progress that has been made in FY 2011, including a review of the modeling approach and parameter data sets (Section A-2), as well as a preliminary evaluation of a newly proposed modeling approach (Section A-3). The summary and a discussion of future work are given in Section A-4.

A-2. Diffusion through Clay Rock: A Review

This section presents a review of approaches to modeling diffusion processes in natural clay formations, and parameter data obtained from relevant experimental observations.

A-2.1 Review of Modeling Approach

Modeling of diffusive transport in clay rocks (natural system) is complicated by the existence of heterogeneity at different scales and coupling between diffusive and electrochemical processes (Revil and Leroy 2004; Appelo et al. 2010; Bourg et al. 2003; Jougnot et al. 2009). At a local scale, different pore spaces co-exist within a representative elementary volume, or a "point" within the context of continuum mechanics. They include pore spaces surrounded by grains other than clay, pore spaces surrounded by clay and other grains, pore spaces surrounded by clay grains only, and interlayer spaces within clay grains. The dominant transport processes of radionuclides can be quite different for these different kinds of pore spaces. For example, the coupling between diffusive and electrochemical processes, or the interaction between diffusion in bulk fluid and an electrical double-diffusion layer near clay surfaces, is negligible for pores surrounded by other grain particles, but critical for small pores surrounded by clay particles and interlayer spaces. The last two pore-space types are especially important for compacted clay systems (such as clay buffers in Engineered Barrier System (EBS)) and also highly relevant for natural clay rock. Modeling approaches for diffusion differ in their treatment of these different types of pores and in their considerations of the electrochemical processes. In the literature, specifically two kinds of modeling approaches are available for describing diffusive transport in clay materials (Bourg et al. 2003; Revil and Leroy 2004; Appelo et al. 2008; Jougnot et al. 2009; Appelo et al. 2010): the phenomenological approach and the mechanistic approach.

A-2.1.1 Phenomenological Approach

The phenomenological approach, a modeling approach based on Fick's diffusion law, uses semi-empirical constants to roughly incorporate the effects of electrochemical processes, such as using the "accessible porosity" to consider anion exclusion effects. While this kind of approach cannot capture detailed transport mechanisms, it is relatively simple, computationally efficient, and straightforward to implement.

Typically, using this approach, the diffusive transport equation is given as:

$$\epsilon R \frac{\partial C}{\partial t} = \nabla \cdot (D_e \nabla C) \qquad \text{Eq. A-1}$$

where C is concentration, t is the time, ϵ is porosity, D_e is effective diffusion coefficient and R is retardation factor which is given by the following equation:

$$R = 1 + \frac{\rho K_d}{\epsilon} \qquad \text{Eq. A-2}$$

where ρ is the dry density of the solid and K_d is the distribution coefficient.

The effective diffusion coefficient is treated as an empirical parameter and is related to the diffusion coefficient of a chemical species in free water by the following equation (e.g., Appelo and Wersin 2007; Appelo et al. 2010):

$$D_e = \epsilon D_p = \epsilon \frac{\delta}{\theta^2} D_w \qquad \text{Eq. A-3}$$

where D_p is the pore-water diffusion coefficient, D_w is the diffusion coefficient in free water, θ^2 is the tortuosity factor, which accounts for the fact that diffusing molecules must pass around solid grains and take a longer path than a straight-line distance, and δ is the constrictivity factor, encompassing the effect of pore narrowing and widening (Appelo et al. 2010). Because it is difficult to derive θ^2 and δ theoretically, researchers tend to obtain them (or a geometrical factor G ($\frac{1}{G} = \frac{\delta}{\theta^2}$) that combines them) by fitting laboratory or field test data. Some researchers do not even bother to calibrate them; they calibrate effective diffusion coefficient directly.

Equations A-1, A-2, and A-3 are consistent with Equations 4-21, 4-16, and 4-9 respectively. The pore-water diffusion coefficient, D_p, in Equation A-3 is equivalent to the bulk diffusion coefficient, D_b, in Equation 4-9. The geometric factor, $1/G$, in Equation A-3 is equivalent to the tortuosity, τ, in Equation 4-9.

In many cases, Equation A-3 has been observed to underpredict the diffusion of cations (e.g., Bourg et al. 2003). This is often interpreted as resulting from the diffusion of adsorbed species along the solid surface. Therefore, as reviewed by Bourg et al. (2003), a semi-empirical effective "surface diffusion coefficient" was introduced to take this effect into account:

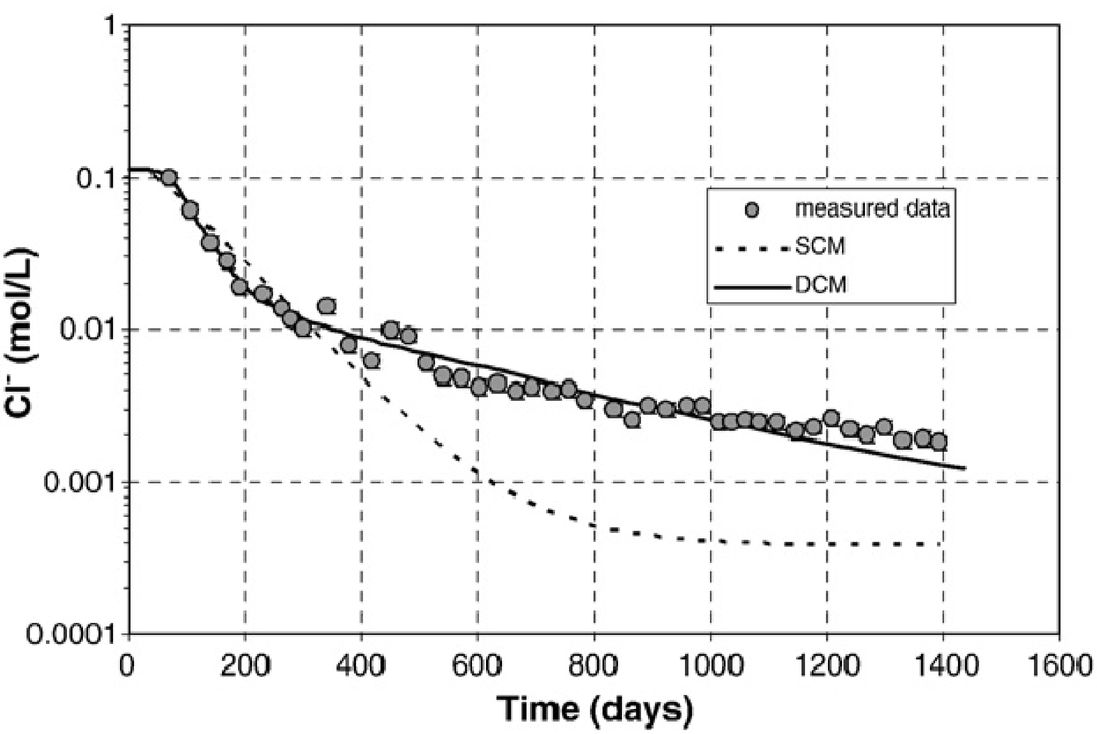
$$D_{e,surf} = \frac{D_{surf} \rho K_d}{\theta^2} \qquad \text{Eq. A-4}$$

where D_{surf} is the so-called surface diffusion coefficient, and subscript e refers to effective parameters throughout this report. The derivation of Equation A-4 was based on an assumption that tortuosity factors are the same for pore space and surface paths (Bourg et al. 2003). Note that the summation of effective diffusion coefficients given in Equations A-3 and A-4 should be used in Equation A-1 for cations.

Negative adsorption of anions — electrostatic anion exclusion from the diffuse layer due to the negative charge of the solid — calls for a further adjustment through replacing a geometrical porosity in Equation A-1 by a so-called accessible porosity. The latter is generally smaller than the former, to account for the fact that within clay, as a result of anion exclusion, a fraction of the porosity does not participate in anion diffusion. This concept of accessible porosity is represented in the clay GDS model by the available porosity parameter (see Equations 3.3-2, 3.3-7, 3.3-13, amd 3.3-15).

The phenomenological approach has occasionally been extended by considering different types of pores (pore spaces surrounded by clay versus those surrounded by other grains), resulting in a type of model that is usually referred to as a *dual-continuum* or *dual-porosity* model (Samper et al. 2008c; Zheng and Samper 2011). The dual-continuum model is motivated by limitations in the phenomenological approach based on a single continuum: this approach has failed to interpret some laboratory or field diffusion test results. For example, Figure A-2 shows the breakthrough curve of chloride for a permeation test using FEBEX bentonite (Samper et al. 2008c). Similar behavior was also observed for the diffusion of tritiated water (HTO) in a natural clay sample (OPA) (van Loon and Jakob 2005). Samper et al. (2008c) showed that the single-continuum model with optimal effective diffusion coefficient and accessible porosity, calibrated by an inverse methodology, fails to reproduce the measured long tail of the breakthrough curve of chloride—whereas the dual-continuum model does a better job, as shown in Figure A-2. The dual-continuum model was first developed for matrix-fracture systems (Barenblatt and Zheltov 1960; Pruess and Narasimhan 1985) and later applied to structured natural soil (Gerke and van Genuchten 1993a; 1993b; Gerke and van Genuchten 1996; Ray et al. 1997; Hantush et al. 2000 ; Lichtner 2000; Hantush et al. 2002; Šimunek et al. 2003). When applying such a model to a clay formation or compacted bentonite, the concept is to divide the porous media system into two continua: one associated with the pores surrounded by clay particles, and the other tied with those surrounded by other grains. The division is either arbitrary (Wilson et al. 1992) or based loosely on the physical characteristics of the soil (Ray et al. 1997). Equation A-1 is applied to both continua, and the mass transfer between the two continua are either calculated by solving the mass-transfer equation perpendicular to the flow direction in the continua (Lichtner 2000) or by a lumped transfer term with a first-order (Gerke and van Genuchten 1993a; 1993b) or higher-order form (Zheng and Samper 2011).

In summary, the phenomenological approach is largely based on a conventional approach to model contaminant transport in porous media, one that essentially ignores the effects of details of electrochemical processes. As a result of its computational and conceptual simplicity, this approach seems to be a natural choice for system-level modeling studies. However, some uncertainties exist when applying it to natural clay formations. As reviewed below in Section A-2.2, although reasonable success with this approach has been achieved with calibrated effective parameters, most experiments (including field tests) used to evaluate this approach were conducted at relatively small scales. It remains to be determined if extrapolation of results from small scales to large scales relevant to a clay geological formation will provide results representative of the actual process. This is simply because our knowledge of how electrochemical processes affect large-scale diffusion is still lacking at this point. Furthermore, most of the effective parameters using this approach are not rigorously defined. Care must be taken when applying the measured values for these parameters to situations in which the corresponding conditions are different. For example, accessible porosity is used to account for the impact of anion exclusion. The latter, however, would likely vary with ionic strength and the charge of the anion in question, and therefore cannot be predicted using an adjusted accessible porosity. In other words, estimated values for accessible porosity are not constants, but a function of experimental conditions and may vary with time in a disposal environment where environmental conditions may change.



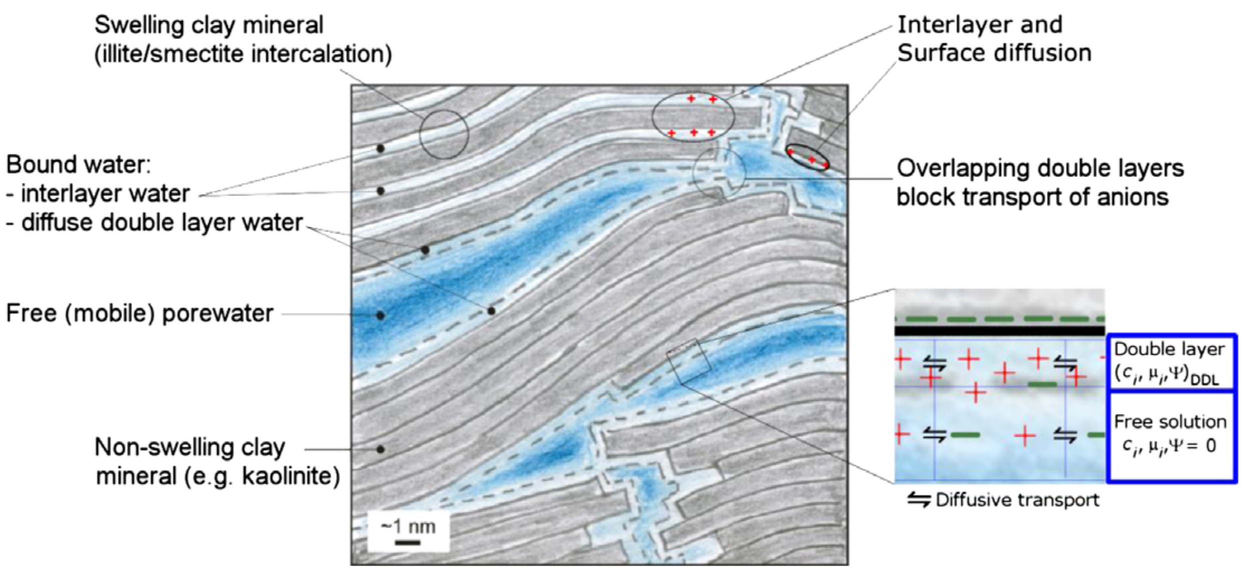
Source: Samper et al. 2008c

Figure A-2. Measured and Computed Breakthrough Curves of Chloride with Single-Continuum Model and Dual-Continuum Model

A-2.1.2 Mechanistic Approach

Mechanistic approaches are based on detailed and explicit descriptions of interactions between diffusion processes and electrochemical processes. Development of improved mechanistic approaches for diffusion processes in clay buffers (bentonite) is an active research activity in the EBS work package. A review of mechanistic approaches within the context of diffusion in bentonite was already provided by Steefel et al. (2010). As a result, we give only a very brief discussion of mechanistic approaches here. However, it is important to note that our interest here is mainly in diffusion within natural clay rock. Although the mechanistic approaches developed for bentonite, in principle, can be applied to natural clay rock, there are some notable differences between features of natural clay rock and bentonite that are relevant to diffusion processes. For example, unlike the EBS bentonite, which contains large proportions of clay minerals (e.g. FEBEX bentonite has 92% of smectite (ENRESA 2000)), clay rock has a relatively small percentage of smectite clay minerals. For example, OPA has only 10% of an illite/smectite mixture (Thury 2002). The pore space surrounded by the clay minerals therefore only accounts for a relatively small portion of whole pore space.

One important feature of clay is that a clay particle's surface is negatively charged, which creates a so-called diffuse double layer (DDL). Figure A-3 presents a schematic diagram of pore space in OPA (Appelo et al. 2010). In a typical pore surrounded by clay, the pore water (close to the surface of the clay) becomes charged by an excess of anions and a deficit of cations, and turns into a DDL. Mechanistic approaches tend to explicitly consider the coupling between diffusive and electrochemical processes, i.e., the diffusion through the free solution and the interaction with DDL (Appelo et al. 2008; Jougnot et al. 2009; Appelo et al. 2010). For example, Appelo et al. (2010) divide water in pore space into three parts, based on their different physical and chemical properties: mobile pore water (that is not impacted by electrochemical processes), DDL water near the pore walls, and interlayer water (occupying spaces between clay layers). Then, the diffusion processes in the three parts and their interactions (or couplings) are modeled.



Source: Appelo et al. 2010

Figure A-3. A Diagram of the Pore Space in OPA Showing
Three Water Types with Associated Diffusion Domains

While a number of mechanistic approaches are available, they are all generally much more complicated than the phenomenological approach and have the following three common features. First, the diffusive flux of a species is the result of both a chemical and electrical potential gradient (Appelo and Wersin 2007). In the other words, the commonly used Fick's law is in general not considered to be applicable anymore. Second, DDL is explicitly incorporated, and the concentrations in DDL are linked to the concentrations in free solution by Boltzmann's equation or Donnan approximation (Appelo and Wersin 2007). Third, the adsorption of ions is calculated by combining a surface complexation model and the DDL (Appelo et al. 2010).

In general, since the electrochemical processes are relatively rigorously considered in a mechanistic approach, this approach does not have the limitations of a phenomenological approach, mentioned in Section A-2.1.1. However, this kind of approach is computationally more complex, involves more parameters, and therefore needs more experimental data to identify parameter values. It may be of interest to indicate that the related parameter values are spatially variable in a natural clay formation, because of the existence of heterogeneity at different scales, which likely increases the burden for parameter determination. This issue, however, may not be a problem for EBS bentonite because, at the continuum scale, heterogeneity for bentonite is minor, as a result of the way it is packed. The related parameter values may also vary temporally, if the clay environment changes chemically or mechanically such as might be caused by changing pore water chemistry or the presence of nuclear materials in a nearby excavation.

A-2.2 Data for Transport Parameters of Clay Formations

This section documents parameter data sets related to diffusion processes in clay formations that are available in the literature**.** In this subsection, "measured parameters" refers to those estimated based on the phenomenological approach (discussed in Section A-2.1.1) from diffusion experiments. Also, while the compilation of the data sets includes typical ones for clay formations, it by no means is exhaustive.

OPA is a geological formation in the northern part of Switzerland with suitable properties for hosting a repository for HLW (Thury 2002). Table A-1 summarizes the measured OPA property values, including effective diffusion coefficients D_e, effective diffusion coefficients in directions parallel and perpendicular to the bedding of clay formation, $D_{e\parallel}$ and $D_{e\perp}$, accessible porosity ε, distribution coefficient K_d, apparent diffusion coefficient D_a, apparent diffusion coefficients in the directions of parallel and perpendicular to the bedding, $D_{a\parallel}$ and $D_{a\perp}$, retardation coefficient *R,* rock capacity factor α and rock capacity factor for directions parallel and perpendicular to the bedding, $\alpha_{\parallel}$ and $\alpha_{\perp}$. As for the entities listed in Table A-1, they are related through the following equations:

$$D_a = \frac{D_e}{\alpha} \qquad \text{Eq. A-5}$$

$$\alpha = \epsilon R \qquad \text{Eq. A-6}$$

Apparently, for nonadsorbed species, Equation A-6 becomes:

$$\alpha = \epsilon \qquad \text{Eq. A-7}$$

Table A-1. Estimated Values of Various Properties for OPA

Species	D_e (m^2/s)	$D_{e\parallel}$ (m^2/s)	$D_{e\perp}$	ε	K_d (mL/g)	D_a (m^2/s)	$D_{a\parallel}$ (m^2/s)	$D_{a\perp}$ (m^2/s)	R	α	$\alpha_{\parallel}$	$\alpha_{\perp}$	Source
HTO	1.36E-11	2.40E-11	3.20E-12	0.16		8.50E-11	1.50E-10	2.00E-11					(Cormenzana et al. 2008)
HTO	3.44E-11	5.60E-11	1.28E-11	0.16		2.15E-10	3.50E-10	8.00E-11					(Cormenzana et al. 2008)
HTO	3.75E-11	6.00E-11	1.50E-11	0.15		2.50E-10	4.00E-10	1.00E-10					(Garcia-Gutierrez et al. 2006)
HTO	3.22E-11	5.00E-11	1.43E-11	0.15		2.14E-10							(Palut et al. 2003)
HTO	1.82E-11	3.10E-11	5.40E-12	1.45E-01		1.26E-10				1.45E-01	0.15	0.14	(Van Loon et al. 2004a)
HTO	1.87E-11	3.20E-11	5.40E-12	1.30E-01		1.44E-10				1.30E-01	0.13	0.13	(Van Loon et al. 2004a)
HTO	3.40E-11	5.40E-11	1.40E-11	1.60E-01		2.13E-10				1.60E-01	0.15	0.17	(Van Loon et al. 2004a)
HTO	3.40E-11	5.40E-11	1.40E-11	1.55E-01		2.19E-10				1.55E-01	0.17	0.14	(Van Loon et al. 2004a)
HTO	4.00E-11	4.00E-11		1.50E-01		2.67E-10				1.50E-01	0.15		(Van Loon et al. 2004a)
HTO	4.00E-11			0.15		2.67E-10							(Van Loon et al. 2004b)
HTO	6.00E-11			0.15		4.00E-10							(Wersin et al. 2008)
HTO	6.70E-12			0.15		4.47E-11							(Van Loon et al. 2003b)
HTO	5.90E-12			0.14		4.21E-11							(Van Loon et al. 2003b)
HTO	5.60E-12			0.13		4.31E-11							(Van Loon et al. 2003b)
HTO	1.50E-11			0.1		1.50E-10							(Van Loon et al. 2003a)
HTO	1.20E-11			0.1		1.20E-10							(Van Loon et al. 2003a)
D2O	2.50E-11	4.00E-11	1.00E-11	0.15									(Samper et al. 2006)
Cl	2.50E-12	4.00E-12	1.00E-12	8.06E-02		3.10E-11	5.00E-11	1.20E-11					(Garcia-Gutierrez et al. 2006)
Cl	9.10E-13			0.044									(Van Loon et al. 2003b)

Table A-1. Estimated Values of Various Properties for OPA (continued)

Species	D_e (m²/s)	$D_{e\parallel}$ (m²/s)	$D_{e\perp}$	ε	K_d (mL/g)	D_a (m²/s)	$D_{a\parallel}$ (m²/s)	$D_{a\perp}$ (m²/s)	*R*	α	$\alpha_{\parallel}$	$\alpha_{\perp}$	Source
Cl	7.90E-13			0.039									(Van Loon et al. 2003b)
Cl	7.10E-13			0.039									(Van Loon et al. 2003b)
Cl	5.70E-12			0.073									(Van Loon et al. 2003a)
Cl	4.10E-12			0.072									(Van Loon et al. 2003a)
Cl	2.04E-12	3.40E-12	6.70E-13	4.50E-02						4.50E-02	0.05	0.04	(Van Loon et al. 2004a)
Cl	1.01E-11	1.60E-11	4.10E-12	8.00E-02						8.00E-02	0.08	0.08	(Van Loon et al. 2004a)
Cl[a]	1.80E-11	1.80E-11		1.00E-01						1.00E-01	0.1		(van der Kamp and Van Stempvoort 1998)
Cl[a]	5.60E-11	5.60E-11		1.50E-01						1.50E-01	0.15		(van der Kamp and Van Stempvoort 1998)
I	5.17E-12	8.27E-12	2.07E-12	8.00E-02									(Samper et al. 2006)
I	6.60E-13			0.083									(Van Loon et al. 2003b)
I	5.00E-13			0.063									(Van Loon et al. 2003b)
I	4.50E-13			0.076									(Van Loon et al. 2003b)
I	4.80E-12			0.105									(Van Loon et al. 2003a)
I	3.40E-12			0.077									(Van Loon et al. 2003a)
I	1.00E-11	1.00E-11		0.09							0.09		(Van Loon et al. 2004a)
I	1.00E-11			0.085									(Van Loon et al. 2004b)
Br^- [a]	1.70E-11	1.70E-11		0.1							0.1		(van der Kamp and Van Stempvoort 1998)
Br^- [a]	4.50E-11	4.50E-11		0.15							0.15		(van der Kamp and Van Stempvoort 1998)
Na	4.55E-11					4.55E-11	7.80E-11	1.30E-11		1.00E+00	0.89	1.11	(Van Loon et al. 2004a)
Na	2.39E-11					4.35E-11	7.20E-11	1.50E-11		5.50E-01	0.62	0.48	(Van Loon et al. 2004a)

Table A-1. Estimated Values of Various Properties for OPA (continued)

Species	D_e (m²/s)	$D_{e\parallel}$ (m²/s)	$D_{e\perp}$	ε	K_d (mL/g)	D_a (m²/s)	$D_{a\parallel}$ (m²/s)	$D_{a\perp}$ (m²/s)	*R*	α	$\alpha_\parallel$	$\alpha_\perp$	Source
Na	3.84E-11					6.00E-11	6.00E-11			6.40E-01	0.64		(Van Loon et al. 2004a)
Na	6.00E-11									0.64			(Van Loon et al. 2004b)
Cs	1.35E-09					1.90E-13			1.92E+04	7.10E+03			(Maes et al. 2008)
Cs	4.05E-10					1.62E-13			6.80E+03	2.50E+03			(Maes et al. 2008)
Cs	1.10E-10					1.00E-13			2.90E+03	1.10E+03			(Maes et al. 2008)
Cs	2.00E-10								$s = 0.186c^{0.53}$				(Van Loon et al. 2004b)
Np(v)	6.90E-12			0.15	0.1					243			(Wu et al. 2009)

NOTE: [a]The measured effective diffusion coefficient and accessible porosity are cited in Van Loon et al. (2004a).

The values directly reported in the corresponding references are shown in the cell with white background, and those with the blue background are derived according to Equations A-5 to A-7.

D_e (m²/s) = effective diffusion coefficient

$D_{e\parallel}$ (m²/s) = effective diffusion coefficient in the direction parallel to the clay-formation bedding

$D_{e\perp}$ (m²/s) = effective diffusion coefficient in the direction perpendicular to the clay-formation bedding

ε = accessible porosity

K_d (mL/g) = distribution coefficient

D_a (m²/s) = apparent diffusion coefficient

$D_{a\parallel}$ (m²/s) = apparent diffusion coefficient in the direction parallel to the bedding

$D_{a\perp}$ (m²/s) = apparent diffusion coefficient in the direction perpendicular to the bedding

R = retardation coefficient

α = rock capacity factor

$\alpha_\parallel$ = rock capacity factor in the direction parallel to the bedding of other clay formations

$\alpha_\perp$ = rock capacity factor in the direction perpendicular to the bedding of other clay formations

In Table A-1, the values directly reported in the corresponding references are shown in the cell with white background, and those with blue background are derived according to Equations A-5 to A-7. To make the inter-reference comparison, two difficulties need to be overcome. First, different researchers chose different type of parameters to report. For example, Cormenzana et al. (2008) reported the accessible porosity and apparent diffusion coefficients for HTO, whereas Van Loon et al. (2004a) reported the rock capacity factor and effective diffusion coefficients for HTO. Second, diffusion processes through the OPA exhibit anisotropy, with a diffusion coefficient parallel to clay-formation bedding that is higher than that perpendicular to the bedding. When conditions allowed—for example, as 3D laboratory or *in situ* data became available for model calibrations—values for diffusion coefficient and rock capacity factor in both directions ($D_{e\parallel}$ and $D_{e\perp}$) were reported (Van Loon et al. 2004a; Garcia-Gutierrez et al. 2006; Samper et al. 2008a). On the contrary, most in- or through-diffusion tests do not allow for calibration of the anisotropic diffusion coefficients (Van Loon et al. 2003a; Van Loon et al. 2003b; Maes et al. 2008; Wersin et al. 2008; Wu et al. 2009), and single values for the diffusion coefficient (D_e) were reported.

We therefore make the following adjustment to make different sets of data comparable. First, we use the effective diffusion coefficient, accessible porosity, and rock capacity factors as the parameters to be compared. For example, if apparent diffusion coefficients are reported (D_a), they are converted to an effective diffusion coefficient (D_e). Second, we take $D_e = (D_{e\parallel} + D_{e\perp})/2$ to overcome the difficulty when anisotropic effective-diffusion coefficients are reported in one reference while isotropic ones are reported in other references. Table A-2 presents values for the maximum, minimum, and average for effective diffusion coefficient, accessible porosity, and rock capacity factor. The diffusion coefficient of HTO has been measured quite extensively. The accessible porosity for HTO is usually close to the physical porosity of OPA and represents the upper bound of diffusive porosity for other species. The difference between minimum and maximum diffusion coefficient of HTO is about one order of magnitude. Accessible porosity for HTO ranges from 0.1 to 0.16, with most values reported around 0.15 (Table A-1). Only the effective diffusion coefficient and accessible porosity of D_2O (deuterium) are reported in Samper et al. (2006), which are calibrated from a 3D model based on the DI-B *in situ* test for OPA. They are quite close to those values for HTO. It is known that chloride is subject to anion exclusion and has an accessible porosity smaller than that for a neutral species such as HTO. As shown in Table A-2, the accessible porosity for chloride ranges from 0.039 to 0.081, with an average of 0.059,

Table A-2. Minimum, Maximum, and Average Values for the Effective Diffusion Coefficient D_e, Accessible Porosity ε, and Rock Capacity Factor α for OPA

Species	D_e **(m²/s)**			ε			α		
	Min	**Max**	**Average**	**Min**	**Max**	**Average**	**Min**	**Max**	**Average**
HTO	5.60E-12	6.00E-11	2.55E-11	0.100	0.160	0.143			
D2O			2.50E-11			0.150			
Cl	7.10E-13	1.01E-11	3.35E-12	0.039	0.081	0.059			
I	4.50E-13	1.00E-11	4.37E-12	0.063	0.105	0.082			
Br	1.70E-11	4.50E-11	3.10E-11	0.100	0.150	0.130			
Na	2.39E-11	6.00E-11	4.20E-11				0.55	1	0.708
Cs	1.10E-10	1.35E-09	5.16E-10				1100	7100	3570
Np(V)			6.90E-12						243

which is about 40% of the porosity for HTO. Because of the smaller accessible porosity, the effective diffusion coefficient for chloride is also smaller, about 13% of that for HTO. The measured effective diffusion coefficient for chloride varies significantly, with a difference between minimum and maximum values that is more than one order of magnitude.

Iodide has slightly higher accessible porosity than chloride, probably because iodide is weakly adsorbed (Savoye et al. 2006a). The average effective diffusion coefficient for iodide is also slightly higher than that for chloride. Only diffusion coefficient and accessible porosity for bromide are reported in Van der Kamp and Van Stempvoort (1998), cited in Van loon et al. (2004b), and both are much higher than those for chloride and iodide, which leads to questioning the reliability of the data. For cations, Table A-2 lists values for the rock capacity factor instead of accessible porosity, because cations are usually adsorbed. The measured effective diffusion coefficient for sodium is quite consistent with the ratio of the maximum to the minimum (2.5), based on the four data points from Van Loon et al. (2004a; 2004b). The average effective diffusion coefficient is about 1.6 fold that of HTO. Sodium is not very strongly adsorbed. Its rock capacity factor ranges from 0.55 to 1 and the average is 0.7. Cesium, on the other hand, is very strongly adsorbed and has an average rock capacity factor of 3570. The large rock capacity factor for cesium leads to a large effective diffusion coefficient, which is about 20 times higher than that for HTO. Diffusion coefficient and rock capacity data for neptunium (V) was only reported in Wu et al. (2009). The rock capacity factor is lower than that for cesium, but the measured effective diffusion coefficient is much smaller than that for HTO. Note that for highly adsorbed cations, measured concentration or flux data are not very sensitive to the diffusion coefficient, so that the calibrated diffusion coefficient might have rather large uncertainty.

The COx argillite formation is a candidate host rock for disposal of HLW in France. Although diffusion through the COx argillite was not as widely studied as the diffusion through the OPA, several researchers have reported values for related parameters such as diffusion coefficient, accessible porosity, and distribution coefficient for COx argillite. Reported parameters are summarized in Table A-3. The entities derived from originally reported ones are in the cells with blue background, while others are directly taken from the literature. In Table A-3, reported values for rock capacity factor (called apparent porosity by the authors in the literature) (Descostes et al. 2008) for HTO, chloride, iodide, SeO_3^{-2}, and SO_4^{-2} are taken to be the same as accessible porosity, with the assumption that these neutral and anionic species are not adsorbed. When effective diffusion coefficients in directions parallel and perpendicular to the bedding of clay formation, $D_{e\parallel}$ and $D_{e\perp}$, are reported, the averages of these coefficients are taken when comparing with the D_e (not considering anisotropic diffusion coefficients) reported by others.

Based on the data listed in Table A-3, we calculated the minimum, maximum, and average for effective diffusion coefficient D_e, accessible porosity ε, and distribution coefficient K_d for COx argillite (Table A-4). The effective diffusion coefficients of HTO for COx are quite consistent from different sources, ranging from 1.1e-11 to 4.9e-11 m^2/s, with an average of 3.1e-11 m^2/s. The accessible porosities of HTO for COx, however, show rather large variations, with a range from 0.15 to 0.25, partially because of some large values reported in Descostes et al. (2008). Descostes et al. (2008) measured the porosity of COx argillite samples taken from different depths of a core. The compositional difference (for example, between the content of clay) might be the possible reason for such variations in porosity. Note that the porosity value reported by Garcia-Gutierrez et al. (2008) (Table A-3) is obtained by the measurement of dry density and grain density. The steady-state concentration profiles collected in Garcia-Gutierrez et al. (2008) from through-diffusion and in-diffusion do not allow for calibration of porosity. The effective diffusion coefficient of chloride for COx seems to exhibit large variation, with a minimum value of 4.8e-13 m^2/s and a maximum value that is about 20 times the minimum one. However, if we leave out 4.8e-13 m^2/s from Descostes et al. (2008), the rest are quite consistent, ranging from 4.4e-12 to 9.1e-12 m^2/s. (The reliability of the measured value of 4.8e-13 m^2/s needs to be further examined). The accessible porosity of chloride ranges from 0.05 to 0.09, with an average of 0.07. The effective diffusion

Table A-3. Estimated Values of Various Properties for COx Argillite

Species	D_e (m²/s)	$D_{e\parallel}$ (m²/s)	$D_{e\perp}$ (m²/s)	ε	K_d (mL/g)	$D_{a\parallel}$ (m²/s)	α	Source
HTO	1.1E-11			0.204			0.204	(Descostes et al. 2008)
HTO	4.4E-11			0.215			0.215	(Descostes et al. 2008)
HTO	3.3E-11			0.165			0.165	(Descostes et al. 2008)
HTO	4.7E-11			0.224			0.224	(Descostes et al. 2008)
HTO	4.9E-11			0.217			0.217	(Descostes et al. 2008)
HTO	1.4E-11			0.171			0.171	(Descostes et al. 2008)
HTO	2.5E-11			0.167			0.167	(Descostes et al. 2008)
HTO	2.7E-11			0.247			0.247	(Descostes et al. 2008)
HTO	1.88E-11	3.00E-11	7.50E-12	0.15				(Garcia-Gutierrez et al. 2008)
HTO	2.93E-11	4.50E-11	1.35E-11	0.15				(Garcia-Gutierrez et al. 2008)
HTO	1.78E-11			0.15				(Garcia-Gutierrez et al. 2008)
HTO	4.22E-11			0.15				(Garcia-Gutierrez et al. 2008)
HTO	3.75E-11			0.15				(Garcia-Gutierrez et al. 2008)
HTO	3.97E-11			0.15				(Garcia-Gutierrez et al. 2008)
HTO	4.10E-11			0.18				(Samper et al. 2008b)
HTO	2.74E-11	4.04E-11	1.45E-11					(Samper et al. 2008b)
HTO	3.06E-11	4.51E-11	1.61E-11					(Samper et al. 2008b)
Cl	4.8E-13			0.049			0.049	(Descostes et al. 2008)
Cl	5.9E-12			0.064			0.064	(Descostes et al. 2008)
Cl	8.4E-12			0.077			0.077	(Descostes et al. 2008)
Cl	4.6E-12			0.065			0.065	(Descostes et al. 2008)
Cl	4.44E-12							(Garcia-Gutierrez et al. 2008)
Cl	8.86E-12							(Garcia-Gutierrez et al. 2008)
Cl	6.48E-12							(Garcia-Gutierrez et al. 2008)
Cl	8.01E-12							(Garcia-Gutierrez et al. 2008)
Cl	9.10E-12			0.09				(Samper et al. 2008b)

Table A-3. Estimated Values of Various Properties for COx Argillite (continued)

Species	D_e (m^2/s)	$D_{e\parallel}$ (m^2/s)	$D_{e\perp}$ (m^2/s)	ε	K_d (mL/g)	$D_{a\parallel}$ (m^2/s)	α	Source
I	2.3E-12			0.284			0.284	(Descostes et al. 2008)
I	4.7E-12			0.065			0.065	(Descostes et al. 2008)
I	4.6E-12			0.053			0.053	(Descostes et al. 2008)
I	1.6E-12			0.033			0.033	(Descostes et al. 2008)
I	4.40E-12			0.13				(Samper et al. 2008b)
SeO_3^{2-}	1E-14			0.003			0.003	(Descostes et al. 2008)
SeO_3^{2-}	1.5E-13			0.009			0.009	(Descostes et al. 2008)
SO_4^{2-}	2.1E-13			0.107			0.107	(Descostes et al. 2008)
SO_4^{2-}	1.9E-12			0.307			0.307	(Descostes et al. 2008)
Na	2.75E-11			0.15	0.37			(Garcia-Gutierrez et al. 2008)
Na	6.09E-11			0.15	0.37			(Garcia-Gutierrez et al. 2008)
Na	6.70E-11			0.18	0.74			(Samper et al. 2008b)
Sr	7.06E-12				0.87			(Garcia-Gutierrez et al. 2008)
Sr	2.63E-13			0.15	0.87	6.00E-13		(Garcia-Gutierrez et al. 2008)
Sr	8.77E-13			0.15	0.87	2.00E-12		(Garcia-Gutierrez et al. 2008)
Sr	2.70E-11	2.70E-11		0.16	1.09			(Samper et al. 2008b)
Cs	3.60E-10			0.18	50			(Samper et al. 2008b)

NOTE: The values directly reported in the corresponding references are shown in the cell with white background, and those with the blue background are derived according to Equations A-5 to A-7.

D_e (m^2/s) = effective diffusion coefficient

$D_{e\parallel}$ (m^2/s) = effective diffusion coefficient in the direction parallel to the clay-formation bedding

$D_{e\perp}$ (m^2/s) = effective diffusion coefficient in the direction perpendicular to the clay-formation bedding

ε = accessible porosity

K_d (mL/g) = distribution coefficient

$D_{a\parallel}$ (m^2/s) = apparent diffusion coefficient in the direction parallel to the bedding

α = rock capacity factor

Table A-4. Minimum, Maximum, and Average Values for Effective Diffusion Coefficient D_e, Accessible Porosity ε, Distribution Coefficient K_d for COx Argillite

Species	D_e (m²/s)			ε			K_d (mL/g)		
	Min	Max	Average	Min	Max	Average	Min	Max	Average
HTO	1.10E-11	4.90E-11	3.14E-11	0.150	0.247	0.179			
Cl	4.80E-13	9.10E-12	6.25E-12	0.049	0.090	0.069			
I	1.60E-12	4.70E-12	3.52E-12	0.033	0.284	0.113			
SeO_3^{2-}	1.00E-14	1.5E-13	8.00E-14	0.003	0.009	0.006			
SO_4^{2-}	2.10E-13	1.90E-12	1.055E-12	0.107	0.307	0.207			
Na	2.75E-11	6.70E-11	5.18E-11	0.15	0.18	0.16	0.37	0.74	0.49
Sr	2.63E-13	2.70E-11	8.80E-12			0.15			0.87
Cs			3.60E-10			0.18			50

coefficients of iodide show small variation, whereas the accessible porosity does not. Again, we call attention to the abnormally large ε value of 0.284 from Descostes et al. (2008). Also reported in Descostes et al. (2008) are the diffusion coefficients and accessible porosities for SeO_3^{-2} and SO_4^{-2}. Some notable observations from these data are (1) the low effective diffusion coefficient, especially for SeO_3^{-2}, which seems to suggest that the bivalent anions have a lower diffusion coefficient than monovalent ones; and (2) the low accessible porosity for SeO_3^{-2} (about one order of magnitude smaller than that for chloride), which seems to suggest that bivalent anions suffer a more significant anion exclusion effect than monovalent, although the accessible porosity for SO_4^{-2} does not show this behavior. It should be noticed that iodide and SO_4^{-2} are weakly adsorbed—the accessible porosity values listed in Table A-4 really are those for rock capacity factor, a product of accessible porosity and retardation factor—which explains why those values are higher. Parameters for three cations—sodium, strontium and cesium—have been reported. Their accessible porosities are similar to that for HTO, all of them are adsorbed, and their diffusion coefficients are not always larger than that for HTO. The values for the effective diffusion coefficients of sodium and cesium are larger than that for HTO, whereas that for strontium is lower.

Diffusion parameters for the Toarcian clayey formation at the Tournemire experimental site (France) have been studied by several researchers (Patriarche et al. 2004b; Savoye et al. 2006b; Motellier et al. 2007). The Tournemire site is a French experimental site chosen by the Institute for Radioprotection and Nuclear Safety to evaluate the migration processes of chemical species through an argillaceous formation (argillites), similar to those studied elsewhere for radioactive waste disposal. Table A-5 lists the measured effective diffusion coefficients D_e, accessible porosity ε, and distribution coefficient K_d, for the Toarcian clayey formation, while Table A-6 summarizes the minimum, maximum, and average values for the effective diffusion coefficient D_e, accessible porosity ε, distribution coefficient K_d. Motellier et al. (2007) measured the effective diffusion coefficients of HTO for several samples under different conditions: with and without fractures or in different orientations. Measured data are quite consistent except for two smaller values: 7.5e-12 and 7.9e-12, which are measured from an orientation 90° to the horizontal direction (not necessarily perpendicular to the clay-formation bedding). As for parameters listed in Table A-6 for chloride, iodide, and bromide, note the large variation in the accessible porosity for iodide and the weak adsorption of iodide.

Table A-5. Estimated Values for Effective Diffusion Coefficients D_e , Accessible Porosity ε , and Distribution Coefficient K_d for Toarcian Clayey Formation (TOc) at the Tournemire Experimental Site (France)

Species	D_e (m^2/s)	ε	K_d (mL/g)	Source
HTO	2.64E-11	0.124		(Motellier et al. 2007)
HTO	2.65E-11	0.124		(Motellier et al. 2007)
HTO	2.83E-11	0.124		(Motellier et al. 2007)
HTO	2.62E-11	0.124		(Motellier et al. 2007)
HTO	2.62E-11	0.124		(Motellier et al. 2007)
HTO	2.75E-11	0.124		(Motellier et al. 2007)
HTO	2.85E-11	0.124		(Motellier et al. 2007)
HTO	2.05E-11	0.124		(Motellier et al. 2007)
HTO	2.06E-11	0.124		(Motellier et al. 2007)
HTO	7.50E-12[a]	0.124		(Motellier et al. 2007)
HTO	7.9E-12[a]	0.124		(Motellier et al. 2007)
HTO	2.22E-11	0.124		(Motellier et al. 2007)
HTO	2.71E-11	0.124		(Motellier et al. 2007)
HTO	3.1E-11	0.124		(Motellier et al. 2007)
HTO	3.36E-11	0.124		(Motellier et al. 2007)
HTO	2.33E-11	0.124		(Motellier et al. 2007)
HTO	2.01E-11	0.124		(Motellier et al. 2007)
Cl	2.20E-12	0.02		(Savoye et al. 2006b)
Cl	3.80E-12	0.02		(Savoye et al. 2006b)
Cl	3.90E-12	0.03		(Savoye et al. 2006b)
Cl	2.60E-12	0.037		(Savoye et al. 2006b)
Cl	3.60E-12	0.037		(Savoye et al. 2006b)
Cl	4.20E-12	0.037		(Savoye et al. 2006b)
Cl	7.50E-12	0.038		(Savoye et al. 2006b)
Cl	4.10E-12	0.042		(Savoye et al. 2006b)
Cl	1.20E-12	0.02		(Patriarche et al. 2004b)
Cl	1.30E-12	0.021		(Patriarche et al. 2004b)
Cl	1.70E-12	0.02		(Patriarche et al. 2004b)
I	2.10E-12	0.037	0.00E+00	(Savoye et al. 2006b)
I	3.00E-12	0.037	0.00E+00	(Savoye et al. 2006b)
I	1.10E-11	0.12	3.50E-02	(Savoye et al. 2006b)
I	9.80E-12	0.14	3.50E-02	(Savoye et al. 2006b)
I	8.00E-12	0.16	5.50E-02	(Savoye et al. 2006b)

Table A-5. Estimated Values for Effective Diffusion Coefficients D_e, Accessible Porosity ε, and Distribution Coefficient K_d for Toarcian Clayey Formation (TOc) at the Tournemire Experimental Site (France) (continued)

Species	D_e (m²/s)	ε	K_d (mL/g)	Source
I	1.60E-11	0.2	6.40E-02	(Savoye et al. 2006b)
I	1.50E-11	0.21	6.70E-02	(Savoye et al. 2006b)
I	2.00E-11	0.25	8.20E-02	(Savoye et al. 2006b)
Br	2.00E-12	0.042		(Savoye et al. 2006b)
Br	3.10E-12	0.05		(Savoye et al. 2006b)
Br	3.40E-12	0.048		(Savoye et al. 2006b)
Br	3.40E-12	0.038		(Savoye et al. 2006b)

NOTE: [a] Measured in an orientation 90° to horizontal.

The values directly reported in the corresponding references are shown in the cell with white background, and those with the blue background are derived according to Equations A-5 to A-7.

Table A-6. Minimum, Maximum, and Average Values for the Effective Diffusion Coefficient D_e, Accessible Porosity ε, Distribution Coefficient K_d for TOc at the Tournemire Experimental Site (France)

Species	D_e (m²/s)			ε			K_d (mL/g)		
	Min	Max	Ave	Min	Max	Ave	Min	Max	Ave
HTO	7.50E-12	3.36E-11	2.37E-11			0.124			
Cl	1.20E-12	7.50E-12	3.28E-12	0.020	0.042	0.029			
I	2.10E-12	2.00E-11	1.06E-11	3.70E-02	2.50E-01	1.44E-01	0.00E+00	2.50E-01	4.23E-02
Br	2.00E-12	3.40E-12	2.98E-12						

As a result of subsurface heterogeneity, diffusion properties vary for a given species within the same clay formation. Effective diffusion coefficient, accessible porosity, and distribution coefficient for the same chemical species also change according to the type of clay formation. So far, data have been compiled for three types of clay formation: OPA, COx argillite, and Toarcian clayey. Table A-7 shows variations in the effective diffusion coefficient among these formations. The large ratios of the maximum value to the minimum value show the significant variability in effective diffusion coefficient. The ratio for HTO associated with OPA is about 10. For the rest of the species, the largest ratio is 22 for iodide associated with OPA, and smallest one is 2.4 for sodium associated with COx. Unlike the diffusion coefficient calibrated from the measured concentration (or flux) data from a diffusion test, the accessible porosity for HTO, usually assumed to be the total porosity, can be measured directly (e.g., by measuring nitrogen or mercury adsorption) or indirectly (e.g., by measuring the dry density and grain density). Therefore, the accessible porosity for HTO has relatively small variation (Table A-8). However, the accessible porosity of chloride and iodide (that is subject to anion exclusion) must be calibrated and therefore has the larger porosity ratio of the maximum to minimum values, up to 7 for iodide (Table A-8). Note that iodide can also be adsorbed.

There are several reasons for the variations in measured diffusion parameters within a given species and clay formation. First, the consistency between results from different types of laboratory and field diffusion tests (such as percolation experiments, pulse injections, through-diffusion and in-diffusion tests) is a concern (Aertsens et al. 2008). Second, the spatial heterogeneity of a clay formation is an important source of variation in parameters. Samples taken from different locations or tests conducted at different places can lead to quite different results. For example, *in situ* tests DI-A2 (Wersin et al. 2008) and DI-A1 (Van Loon et al. 2004a) have the same setup but are located 1 m apart. The diffusion coefficients for HTO, I- and Cs+ are quite different for these two tests. Third, the anisotropy of a given clay sample apparently can cause variation in parameters along different directions (e.g., Cormenzana et a. 2008; Van Loon et al. 2004a; Motellier et al. 2007).

Table A-7. Values for Effective Diffusion Coefficient (m^2/s) of Different Species for OPA, COx Argillite, and TOc

Clay Rock	HTO		Cl		I		Br		Na		Cs	
	Max /Min	Average	Max /Min	Average	Max /Min	Average	Max /Min	Average	Max /Min	Average	Max /Min	Average
OPA	10.7	2.55E-11	14.2	3.35E-12	22.2	4.37E-12	2.69	3.1E-11	2.5	4.2E-11	12.2	5.16E-10
COx	4.4	3.14E-11	18.92	6.25E-12	2.9	3.52E-12			2.4	5.18E-11		3.6E-10
TOc	4.5	2.37E-11	6.3	3.28E-12	9.5	1.06E-11	9.5	2.98E-12				

Table A-8. Values for Accessible Porosity of Different Species for OPA, COx Argillite, and TOc

Clay rock	HTO		Cl		I	
	Max/Min	Average	Max/Min	Average	Max/Min	Average
OPA	1.6	0.14	2.1	0.059	1.7	0.082
COx	1.6	0.18	1.8	0.069	3.9	0.070
TOc		0.12	2.1	0.029	6.8	0.144

A-3. An Improved Modeling Approach

Because of its computational and conceptual simplicity, the phenomenological approach has often been used for analyzing diffusion experiment results (Section A-2.2) and also seems to be a natural choice for system-level modeling of diffusion processes. However, as previously indicated, this approach is subject to a number of limitations, mainly because it does not account for the effects of detailed electrochemical processes. This section presents an improved modeling approach to remove some of these limitations. In particular, our model development focuses on two questions that are fundamental to modeling diffusion processes in natural clay rock (within the context of system-level modeling): (1) Can Fick's law be an acceptable approximation for modeling diffusion? (2) How can essential features of electrochemical processes be incorporated into a simple diffusion model? As discussed later, answers to these questions may be different for dense clay (bentonite) and natural clay rock: our focus here is on the latter.

A-3.1 Theoretical Basis

For simplicity, we divide pore water into two parts: (1) mobile water in macropores that is not subject to electrochemical processes, and (2) pore water with DDL (including interlayers) that is strongly impacted by electrochemical processes. Based on the Donnan approximation, the electrochemical potential of species *i* is given by (Appelo et al. 2010):

$$\mu_{i,D} = \mu_i^0 + RTlna_{i,D} + z_i F\varphi \qquad \text{Eq. A-8}$$

where subscript D refers to average properties within DDL, μ_i^0 is the standard potential, R is the gas constant, T is the absolute temperature, $a_{i,D}$ is the activity, z_i is the charge number, F is Faraday constant, and φ is the electrical potential.

The chemical potential for macropore water, μ_i , is described by

$$\mu_i = \mu_i^0 + RTlna_i \qquad \text{Eq. A-9}$$

where a_i is the activity for the macropore water. It is commonly assumed that at local scale, chemical equilibrium exists (e.g., Appelo et al. 2010; Leroy et al. 2007), or chemical potentials defined in Equations A-8 and A-9 are equal. Therefore, we have from Equations A-8 and A-9

$$a_{i,D} = a_i exp\left\{-\frac{z_i\varphi}{RT}\right\} \qquad \text{Eq. A-10}$$

Based on the general relationship between diffusion flux and gradient of chemical potential (Appelo et al. 2010; Leroy et al. 2007), and considering that the total diffusion flux is the summation of fluxes for macropore water and the DDL, we obtain the total flux:

$$J_i = -f\frac{D_{e,M}C_i}{RT}\nabla\mu_i - (1-f)\frac{D_{e,D}C_{i,D}}{RT}\nabla\mu_{i,D} \qquad \text{Eq. A-11}$$

where f is the volumetric fraction of macropore water in the pore porosity, and C is concentration. $D_{e,M}$ and $D_{e,D}$ are effective diffusion coefficients for macropore space and the DDL, respectively, and can be calculated following Equation A-3. Considering the practical difficulty in determining tortuosity and constrictivity independently for both macropore water and the DDL, we assume here that they are the same as the first order of approximation. In this case, we can derive from Equation A-3:

$$D_{e,M} = D_{e,D} = \frac{D_{e,HTO} D_{w,i}}{D_{w,HTO}} \qquad \text{Eq. A-12}$$

where subscript w refers to the diffusion coefficient in free water, and $D_{e,HTO}$ is the effective diffusion coefficient (defined by Equation A-3) for HTO that is not subject to electrochemical processes.

If we further assume the reactivity coefficient (the ratio of activity to concentration) to be one for both parts of pore water, we obtain the following relationship between diffusive flux and concentration gradient by combining Equations A-9, A-10, and A-11:

$$J_i = -D_{e,M} \left\{ f + (1-f) exp \left[-\frac{z_i \varphi}{RT} \right] \right\} \nabla C_i \qquad \text{Eq. A-13}$$

The derivation of Equation A-13 employs a previously discussed approximation that at local scale, chemical potentials are the same for the DDL and macropore water. One important implication from Equation A-13 is that Fick’s law is still applicable for modeling the diffusion process in natural clay, largely resulting from the fact that macropore water (that is not subject to electro-mechanical process) exists, such that the chemical potential gradient in the two parts of the water can be described by the concentration gradient corresponding to the macropore–water part. This may not be the case for EBS bentonite, in which DDL overlapping may occur, even within a relatively large pore (Steefel et al. 2010).

From Equation A-13, the effective diffusion coefficient can be written as

$$D_{e,i} = D_{e,M} \left\{ f + (1-f) exp \left[-\frac{z_i \varphi}{RT} \right] \right\} \qquad \text{Eq. A-14}$$

Note that in the above equation, the electrical potential may change with the reactive transport process (such as a change in ionic strength). For a natural clay formation, the electrical potential may not change significantly (Jougnot et al. 2009). Therefore, in this study, we assume that potential to be constant.

It is of interest to compare our approach with the commonly used phenomenological approach (Section A-2.1.1). Both approaches calculate diffusion flux using Fick’s law, and consequently our approach has a computational efficiency similar to that of the phenomenological approach. However, our approach explicitly considers the effects of electrochemical processes, although we employed a number of assumptions/approximations, based on the practical consideration that model simplicity is a desirable feature for system-level models.

A-3.2 Preliminary Evaluation

In Section A-3.1, we proposed an improved diffusion model that considers the effects of electrochemical processes through the dependence of an effective diffusion coefficient on electrical properties of clay rock (Equation A-14). In other words, the key element of our approach is Equation A-14, which can be rearranged as

$$\frac{D_{e,i}}{D_{e,M}} = f + (1-f)exp\left[-\frac{z_i\varphi}{RT}\right] \qquad \text{Eq. A-15}$$

Therefore, the evaluation of the approach focuses on examining how Equation A-15 represents parameter values obtained from experimental observations.

Figure A-4 shows a comparison between measured and calculated values for the ratio of diffusion coefficient ($\frac{D_{e,i}}{D_{e,M}}$). The filled and open rectangles in the figure correspond to data points for OPA from Appelo et al. (2010) and Wersin et al. (2008), respectively. These data points represent results for HTO, Cl^-, B_r^-, I^-, Cs^+, N_a^+, $^{85}Sr^{2+}$ and $^{60}Co^{2+}$. To calculate diffusion-coefficient ratio from the data, we calculate $D_{e,M}$ from Equation A-12 with water self-diffusion coefficient, and diffusion coefficient in free water, for a corresponding chemical species determined from Harris and Woolf (1980) and Li and Gregory (1974), respectively.

To calculate the diffusion coefficient ratio using Equation A-15, we treat *f* and $A = \frac{\varphi}{RT}$ as two fitting factors in this study. (While they may be able to be determined independently from relevant data, an acceptable approach for doing so is not yet available in the literature.) The solid curve in the figure is the best match of Equation A-15 to the data for a given *f* = 0.4. The parameter *f* was not further adjusted to optimize the match. The dashed line corresponds to the same A value as the solid line, but a different *f* value (0.2). Differences between these two curves are not considered significant, indicating that the ratio calculated from Equation A-15 is not very sensitive to *f* within a certain range of *f* values. The comparison between calculated and observed results is fairly reasonable, supporting the usefulness of our approach. However, notable differences between observed and calculated ratio values occur for C_S^+ (the three data points with ratio values larger than 3 for $z_i = 1$ in Figure A-4). Note that for highly adsorbed cations like C_S^+, as previously discussed, measured concentration or flux data used to determine diffusion coefficient estimates are not very sensitive to values for the diffusion coefficient, so that the corresponding estimates (or data points in Figure A-4) might have rather large uncertainty. Also, Figure A-4 only includes a few data points for OPA; we are planning to use all the data presented in Section A-2.2 to further evaluate the approach in the future.

To further examine the practical usefulness of incorporating the effects of electrochemical effects into an effective diffusion coefficient, we check whether observed breakthrough curves can be captured by a modeling approach based on Fick's law and treating diffusion coefficient as an uncertain parameter. (The uncertainty partially comes from the treatment of electrochemistry effects.) This is highly relevant to system-level models for diffusion in clay, because they use Fick's law and allow for consideration of parameter uncertainty. We evaluate this issue with results from an *in situ* diffusion test using inert and reactive tracers at the Bure site in France (Samper et al. 2008a).

Andra has undertaken an extensive characterization program at the Bure site to assess the feasibility of a deep HLW repository in the COx. Diffusion of inert and reactive tracers (DIR) is one of several experimental programs that aim at characterizing diffusion and retention of radionuclides in clay rock. Figure A-5 shows the sketch of the experiment. The experiment was an *in situ* single-point dilution test that involved injecting tracers into a 1-m-long packed-off section of the boreholes. Details of the experiment are given in Samper et al. (2008b).

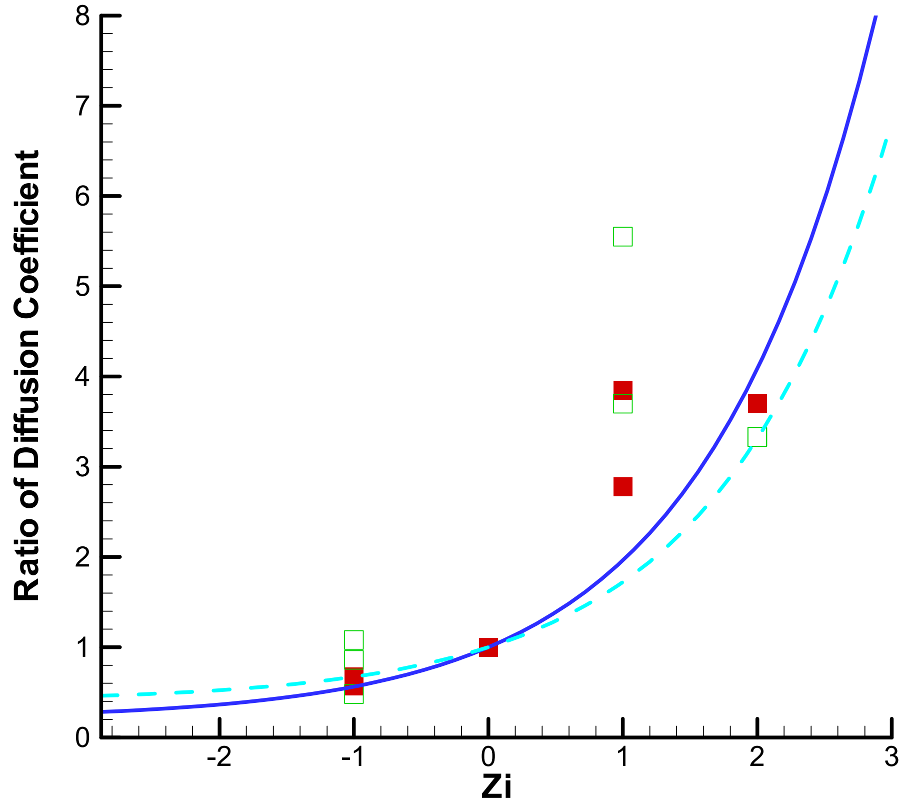
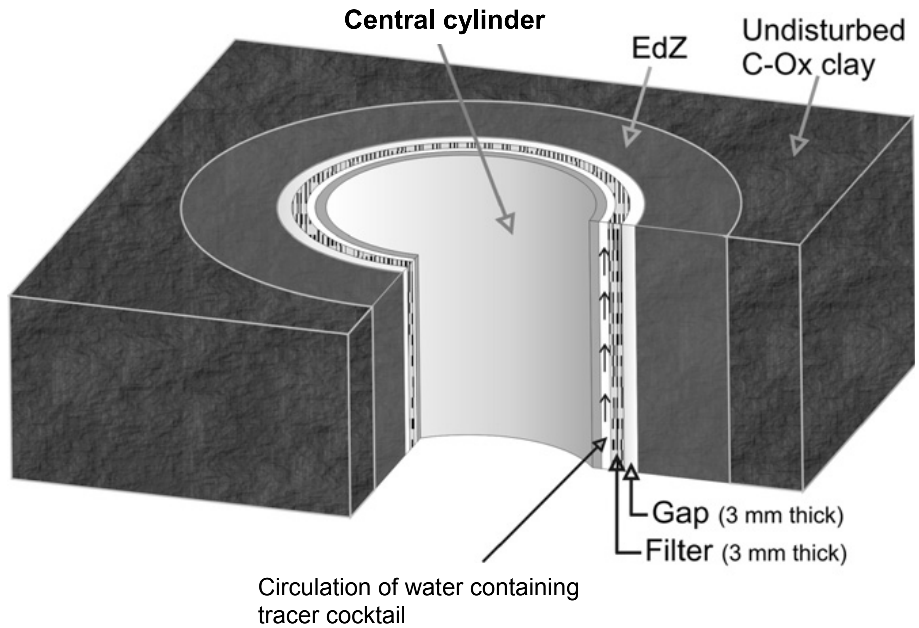


Figure A-4. Comparison between Calculated (Curves) and Observed (Rectangles) Values for Ratio of Diffusion Coefficient as a Function of Charge Number z_i

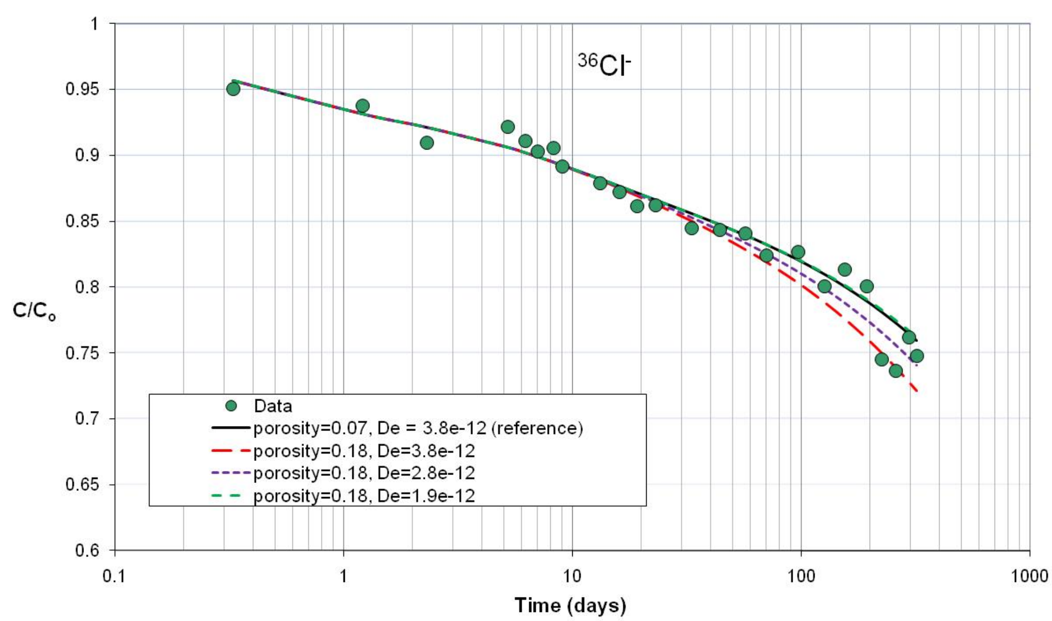
The conventional approach requires calibrating the accessible porosity and effective diffusion coefficient for anions. For this study based on the proposed approach, we use total porosity and the effective diffusion coefficient from Equation A-15. In this report, we use the same numerical model as developed in Samper et al. (2008a). The model uses 2D axi-symmetric finite element mesh and the simulation is conducted with INVERSE-CORE^{2D} (Dai and Samper 2004). Figure A-6 shows the measured chloride concentration, the optimal accessible porosity, and the effective diffusion coefficient. Also shown in Figure A-6 is the model results with total porosity (0.18) and several possible effective diffusion coefficients calculated from Equation A-15. It shows that our approach leads to either very similar results to the reference model, or results within the error of measured data.

Our approach considers the DDL effect by modifying the effective diffusion coefficient but not the adsorption. In other words, the distribution coefficient or retardation factor is still needed when applying our approach. Those model results, shown in Figure A-7, have a distribution coefficient of 1.13 ml/g. We also model the diffusion of sodium (Figure A-7) with two other effective diffusion coefficients: 3.4e-11 m^2/s, which is about 2/3 of the reference value, and 8.5e-12 m^2/s, which is about 1/6 of the reference value. Compared with the reference model, the model with smaller diffusion coefficient deviates from the best fit, but the effect is rather minimal.



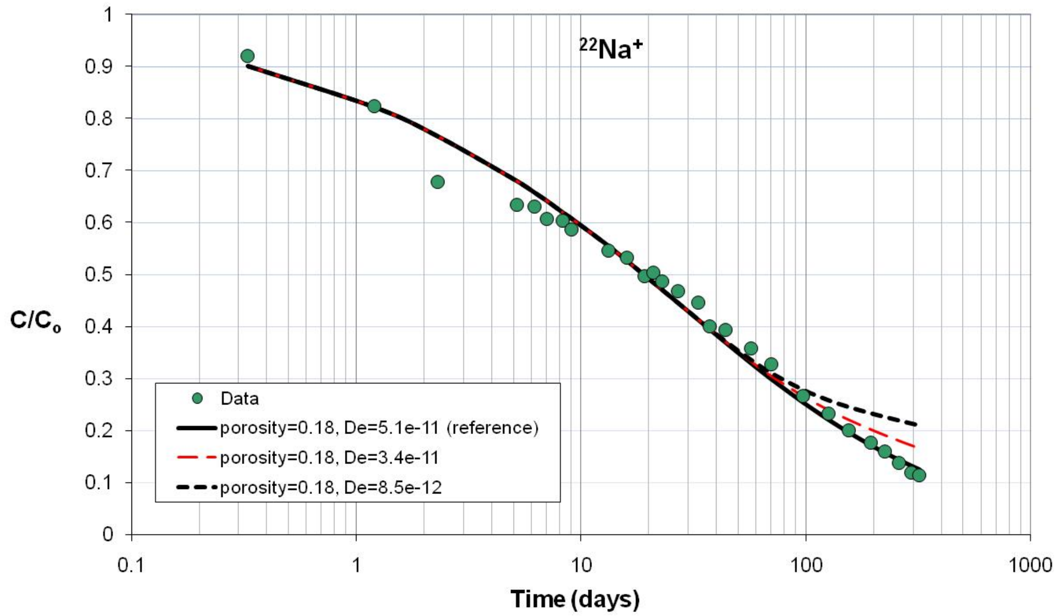
Source: Sampler et al. 2008

Figure A-5. Sketch of Borehole Geometry for DIR Experiments



Source: Measured data (Sampler et al. 2008a)

Figure A-6. Measured and Computed Cl Concentration with Several Effective Diffusion Coefficients (m^2/s)



Source: Measured data (Samper et al. 2008a)

Figure A-7. Measured and Computed Na Concentration with Several Effective Diffusion Coefficients (m^2/s)

A-4. Concluding Remarks

Summary—Diffusion is the dominant mechanism for radionuclide transport in a clay repository under undisturbed conditions. Modeling of diffusive transport in clay rocks is complicated by the existence of heterogeneity at different scales and coupling between diffusive and electro-chemical processes. This report reviews the two kinds of modeling approaches. Phenomenological approaches are based on Fick's diffusion law and use semi-empirical constants to roughly incorporate the effects of electro-chemical processes. While they cannot capture the detailed transport mechanisms and therefore inherently introduce a certain modeling uncertainty, they are relatively simple, computationally efficient, and straightforward to implement. Mechanistic approaches are based on detailed and explicit descriptions of interaction between diffusion processes and electro-chemical processes. They do not suffer the limitations of phenomenological approaches, but are computationally more complex and involve more parameters. This report also reviews and compiles data sets of parameters related to diffusive transport in clay formations that are available in the literature. These data sets provide useful information for evaluating modeling approaches and can be used as inputs into relevant models. An improved modeling approach is proposed to combine the advantages of phenomenological and mechanistic approaches. Results from a preliminary evaluation of the approach are encouraging.

Future Work—The list below describes potential future work in the area of diffusion modeling in clay.

- Continue to evaluate the proposed modeling approach with more data. The approach has been evaluated with a few data points (Figure A-4) and by a comparison between simulation results based on the approach and test observations. More evaluations are needed to improve and/or increase the confidence in the approach.

- Investigate the impact of heterogeneity (and anisotropy) on large-scale diffusion process by comparing simulation results with apparent diffusion coefficients and without considering heterogeneity and those theoretical and numerical results that explicitly consider heterogeneity. The outcome should be useful for determining how the heterogeneity should be treated in system-level modeling of diffusion in clay.
- Integrate process modeling of diffusion in clay with system-level modeling. LBNL will work with ANL to develop process-modeling results to support ANL's system-level diffusion model for clay.
- Study the impact of electrochemical process on large-scale diffusion. As previously indicated, our knowledge of this impact is still lacking. Once a rigorous mechanistic approach is available from the EBS work (e.g., Steefel et al. 2010), we will compare simulation results obtained with our proposed and the mechanistic approaches for a large-scale problem to check how well our approach can capture the large-scale electro-chemical process.

Appendix B

Results of FEPs Mapping

B-1. FEPs Mapping Methodology and Results

As discussed in Section 2, the FEPs mapping activity consists of describing the four individual GDS models for salt, granite, clay, and deep borehole disposal (Section 3) in terms of the relevant FEPs. The goal is to provide the FEPs mapping as an aid to model developers in future GDSM efforts. Using a common framework to document the baseline capabilities of the four individual GDS models increases the transparency and traceability of the technical content of the models. Further, the mapping relies on the UFD list of 208 FEPs documented FY 2010 (Freeze et al. 2010) and updated in FY 2011 (Freeze et al. 2011a). Within the UFD Campaign, these UFD FEPs provide a common context for the identification of knowledge gaps, which can then be prioritized using system-level PA modeling (DOE 2010d, Section 1.2). Accordingly, the use of this common FEPs context for the mapping activity will enhance communication and coordination between the GDSM team and other UFD teams.

In the FEPs FY 2010 progress report (Freeze et al. 2010, Table A-1), the 208 UFD FEPs are characterized by a "UFD FEP Number", "Description", and "Associated Processes". This same information, updated to be consistent with the FY 2011 progress report (Freeze et al. 2011, Table A01) and with slight changes in naming terminology, was included in an MS Excel-based tool developed to facilitate the mapping activity. A description of this information and the related terminology is provided below:

- *UFD FEP Number (called "UFD FEP ID" in the FEPs mapping tool)*—The numbering scheme is based on a hierarchical system that groups similar FEPs together. The numbers associated with various domains, features, events, and processes in Figure 2-1 correspond to the FEP numbering system. Across the disposal system domains there is a consistent structure and numbering scheme for the features (2.x.01 contains the first feature, 2.x.02 contains the second feature, etc.) and the processes (2.x.07 contains mechanical processes, 2.x.08 contains hydrologic processes, etc.).
- *Description (called "UFD FEP Title" in the FEPs mapping tool)*—This item provides a coarse level of detail. The intent is that it be broad enough to be potentially applicable to the full range of disposal system alternatives. For example, "Sorption of Dissolved Radionuclides in the EBS" is potentially relevant to all waste form types and disposal concepts/geologic settings.
- *Associated Processes (called "Process/Issue Description" in the FEPs mapping tool)*—Each FEP is further defined by additional details under "Associated Processes". The level of detail collectively captured by the FEP Descriptions and Associated Processes is appropriate for the current FEP identification step of FEP analysis.

The results of the FEPs mapping activity for the four individual GDS models are located in the following tables: Table B-1 (salt and granite) and Table B-2 clay and deep borehole). The FEPs mapping reflects the Freeze Point 2 versions of the models.

The tables are based on the FEPs mapping tool, which provides three pick-list options for specifying whether a particular FEP is included: yes, partially, no. For mature models in a regulatory environment, a FEP is normally included or excluded. However, at this early stage of model development, the "partially" designation was added to better describe the situation in which only a portion of the capabilities needed to address a FEP have been implemented. There is also a "Description" field (unrelated to the "Description" or "UFD FEP Title" above) for comment or explanation. If a particular FEP is included, the "Description" typically indicates where and how in the model the FEP is included. For partially included FEPs, the entry also indicates what aspects of the FEP are included. For FEPs (or aspects of FEPS) that are not included, the entry may provide additional information such as whether there are plans to include the FEP in the future or whether such inclusion is unlikely. It is important to remember that the capabilities of the individual GDS models are being integrated into the GPAM. Afterwards, improvements to the capability to simulate a particular disposal option, including the inclusion of new FEPs, will be done in GPAM. Therefore, any discussion in the results tables about potentially including a FEP to an individual model should be viewed in the context of adding the FEP to the modeling capability for that disposal option rather than to that specific model.

Unlike the four individual models, the GPAM was not selected for FEPs mapping at this time because of its early stage of development. Moreover, the transition to the GPAM involves incorporating the capability to model all of the FEPs included in the individual GDS models. Consideration can be given to mapping GPAM in the future when it is more stable and the effort more likely to yield useful results. In the meantime, there is a crosswalk showing how aspects of the four individual models are being integrated into GPAM (Table 4-5).

Note that there have been no FEP screening evaluations conducted as yet. The decision to include or exclude a FEP or aspects of a FEP at this point is based solely on the expert opinion of subject matter experts. The current emphasis is on building a PA capability. Screening evaluations can be conducted at some point in the future as the modeling effort evolves to meet the needs of the UFD Campaign and as relevant regulations are identified.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
0.0.00.00	0. ASSESSMENT BASIS					
0.1.02.01	Timescales of Concern		Yes	The simulation runs can be set for 1,000,000 yr as seen in the simulation settings.	Yes	Simulations can be run to 1,000,000 yr.
0.1.03.01	Spatial Domain of Concern		Yes	The spatial domain is specified in multiple model components. Some components make use of parameters defined in other components to calculate dimensions. The following provides pathways to parameters and calculations for the spatial dimensions of different model domains: **Basic Dimensions for Use in Various Domains:** *SaltGDSE_Parameters > WP_Config_data, Salt_GDSE_Data,* and *Salt_GDSE_Config* **Near-Field:** *Near_Field > NearFiled_Config > Salt_NF_volume* **Near-Field Interface:** *NF_Interface > IF_SaltBlock_Transport > Salt_IF_parameters* and *IF_MixingCell_Properties* **Near-Field Marker Bed:** *NF_MB_Transport > NF_MB_Transport > NFMB_MixingCell_Properties* **Far-Field Marker Bed:** *FF_MB_Transport > FFMB_MixingCell_Properties* Note that the salt and granite GDS models are using the same square repository dimensions.	Yes	The physical dimensions of the repository area and of the host rock are implemented at \Container1\near_field_new\Repository_config\GDSE_NF_volume. Physical dimensions of the Far Field are included in the FEHM DLL. The FEHM DLL is implemented at \Container1\Far_Field\FEHM_localize.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
0.1.09.01	Regulatory Requirements and Exclusions		Partially	Some generic elements of the regulatory framework, such as the 1,000,000-yr timescale (FEP 0.1.02.01), are included. However, to the extent that the current framework is specific to Yucca Mountain, it is not applicable to generic modeling of a repository. In addition, there is uncertainty regarding the future framework. Currently, the individual GDS model capabilities are being transitioned into the GPAM. When there is additional clarity in the framework, the GPAM can be analyzed to determine the appropriate changes.	No	Some generic elements of the regulatory framework, such as the 1,000,000-yr timescale (FEP 0.1.02.01), are included. However, to the extent that the current framework is specific to Yucca Mountain, it is not applicable to generic modeling of a repository. In addition, there is uncertainty regarding the future framework. Currently, the individual GDS model capabilities are being transitioned into the GPAM. When there is additional clarity in the framework, the GPAM can be analyzed to determine the appropriate changes.
0.1.10.01	Model Issues	– Conceptual model – Mathematical implementation – Geometry and dimensionality – Process coupling – Boundary and initial conditions	Partially	The current treatment of these modeling issues reflects the fact that a generic, simplified approach has been used to support this early stage of development. The conceptual model informed the model development and is represented with a schematic on the initial screen of the GoldSim file. The file is the mathematical implementation, and the geometry and dimensionality are contained in multiple model components (FEP 0.1.03.01). The current version has only limited coupling among some processes. Closer coupling of processes will be done in future versions. Boundary and initial conditions have been implemented to the extent applicable in the model, some at the model component level and others at the system level.	Partially	The current version of the model includes the first iteration of work on these issues. As such the issues are mostly addressed at a high level. Future iterations of the model will include more refined implementations.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
0.1.10.02	Data Issues	– Parameterization and values – Correlations – Uncertainty	Partially	At this early stage of development, it is important to exercise the model and demonstrate capability. As a result, the forms and values of input parameters simply need to be reasonable representations. In the future when greater rigor is needed, work being done by other parts of the UFD Campaign will be used to inform decisions regarding data issues.	No	At this early stage of development, it is important to exercise the model and demonstrate capability. As a result, the forms and values of input parameters simply need to be reasonable representations. In the future when greater rigor is needed, work being done by other parts of the UFD Campaign will be used to inform decisions regarding data issues.
1.0.00.00	1. EXTERNAL FACTORS					
1.1.00.00	1. REPOSITORY ISSUES					
1.1.01.01	Open Boreholes	– Site investigation boreholes (open, improperly sealed) – Preclosure and postclosure monitoring boreholes – Enhanced flow pathways from EBS	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.1.02.01	Chemical Effects from Preclosure Operations – In EBS – In EDZ – In Host Rock	– Water contaminants (explosives residue, diesel, organics, etc.) – Water chemistry different than host rock (e.g., oxidizing) – Undesirable materials left – Accidents and unplanned events	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
1.1.02.02	Mechanical Effects from Preclosure Operations – In EBS – In EDZ – In Host Rock	– Creation of excavation-disturbed zone (EDZ) – Stress relief – Boring and blasting effects – Rock reinforcement effects (drillholes) – Accidents and unplanned events – Enhanced flow pathways [see also Evolution of EDZ in 2.2.01.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.1.02.03	Thermal-Hydrologic Effects from Preclosure Operations – In EBS – In EDZ – In Host Rock	– Creation of excavation-disturbed zone (EDZ) – Stress relief – Boring and blasting effects – Rock reinforcement effects (drillholes) – Accidents and unplanned events – Enhanced flow pathways [see also Evolution of EDZ in 2.2.01.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.1.08.01	Deviations from Design and Inadequate Quality Control	– Error in waste emplacement (waste forms, waste packages, waste package support materials) – Error in EBS component emplacement (backfill, seals, liner) – Inadequate excavation / construction (planning, schedule, implementation) – Aborted / incomplete closure of repository – Material and/or component defects	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.1.10.01	Control of Repository Site	– Active controls (controlled area) – Retention of records – Passive controls (markers)	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.1.13.01	Retrievability		No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.00.00	2. GEOLOGICAL PROCESSES AND EFFECTS					
1.2.01.00	2.01. LONG-TERM PROCESSES					
1.2.01.01	Tectonic Activity – Large Scale	– Uplift – Folding	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.02	Subsidence		No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.03	Metamorphism	– Structural changes due to natural heating and/or pressure	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.04	Diagenesis	– Mineral alteration due to natural processes	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.05	Diapirism	– Plastic flow of rocks under lithostatic loading – Salt/Evaporites – Clay	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.06	Large-Scale Dissolution		No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
1.2.03.00	2.03.SEISMIC ACTIVITY					
1.2.03.01	Seismic Activity Impacts EBS and/or EBS Components	– Mechanical damage to EBS (from ground motion, rockfall, drift collapse, fault displacement) [see also Mechanical Impacts in 2.1.07.04, 2.1.07.05, 2.1.07.06, 2.1.07.07, 2.1.07.08, and 2.1.07.10]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.03.02	Seismic Activity Impacts Geosphere – Host Rock – Other Geologic Units	– Altered flow pathways and properties – Altered stress regimes (faults, fractures) [see also Alterations and Impacts in 2.2.05.01, 2.2.05.02, 2.2.05.03, 2.1.07.01, and 2.1.07.02]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.03.03	Seismic Activity Impacts Biosphere – Surface Environment – Human Behavior	– Altered surface characteristic – Altered surface transport pathways – Altered Recharge	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.2.04.00	2.04. IGNEOUS ACTIVITY					
1.2.04.01	Igneous Activity Impacts EBS and/or EBS Components	– Mechanical damage to EBS (from igneous intrusion) – Chemical interaction with magmatic volatiles – Transport of radionuclides (in magma, pyroclasts, vents) [see also Mechanical Impacts in 2.1.07.04, 2.1.07.05, 2.1.07.06, 2.1.07.07, and 2.1.07.08]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.04.02	Igneous Activity Impacts Geosphere – Host Rock – Other Geologic Units	– Altered flow pathways and properties – Altered stress regimes (faults, fractures) – Igneous intrusions – Altered thermal and chemical conditions [see also Alterations and Impacts in 2.2.05.01, 2.2.05.02, 2.2.05.03, 2.1.07.01, 2.1.07.02, 2.2.09.03, 2.2.11.06 and 2.2.11.07]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.04.03	Igneous Activity Impacts Biosphere – Surface Environment – Human Behavior	– Altered surface characteristic – Altered surface transport pathways – Altered recharge – Ashfall and ash redistribution	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.3.00.00	3. CLIMATIC PROCESSES AND EFFECTS					
1.3.01.01	Climate Change – Natural – Anthropogenic	– Variations in precipitation and temperature – Long-term global (sea level, …) – Short-term regional and local – Seasonal local (flooding, storms, …) [see also Human Influences on Climate in 1.4.01.01] [contributes to Precipitation in 2.3.08.01, Surface Runoff and Evapotranspiration in 2.3.08.02]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.3.04.01	Periglacial Effects	– Permafrost – Seasonal freeze/thaw	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.3.05.01	Glacial and Ice Sheet Effects	– Glaciation – Isostatic depression – Melt water	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion. The plan is to include sensitivity studies for addressing the effect of future glaciation events on the performance of a generic repository sited in crystalline rock.
1.4.00.00	4. FUTURE HUMAN ACTIONS					
1.4.01.01	Human Influences on Climate – Intentional – Accidental	– Variations in precipitation and temperature – Global, regional, and/or local – Greenhouse gases, ozone layer failure [contributes to Climate Change in 1.3.01.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
1.4.02.01	Human Intrusion – Deliberate – Inadvertent	– Drilling (resource exploration, …) – Mining / tunneling – Unintrusive site investigation (airborne, surface-based, …) [see also Control of Repository Site in 1.1.10.01]	Partially	The salt GDS model considers an undisturbed, or reference, case and a disturbed case representing human intrusion. The GoldSim file for the disturbed case is the same as that for the undisturbed case except for an additional component to implement the stylized human intrusion scenario. In this scenario, a single borehole is assumed to penetrate at 1,000 yr. The number of affected waste packages is sampled with possible values ranging from 1 to 5. Radionuclides from affected waste packages are released directly to an overlying aquifer by pressurized brines with steady-state flow rates. At this time, the model does not consider potential dose impacts of waste brought up by drilling activities.	Partially	The granite GDS model considers an undisturbed, or reference, case and a disturbed case representing human intrusion. In the human intrusion scenario, a single borehole is assumed to penetrate at 1,000 yr. The number of affected waste packages is sampled with possible values ranging from 1 to 5. Radionuclides from affected waste packages are released through a fast pathway to the aquifer. The flow rate up the borehole is a sampled parameter. At this time, the model does not consider potential dose impacts of waste brought up by drilling activities. Parameters relevant to this scenario are defined at \Container1\Human_Intrusion and at \Uncertain_Parameters\HI_parameters.
1.4.11.01	Explosions and Crashes from Human Activities	– War – Sabotage – Testing – Resource exploration / exploitation – Aircraft	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.5.00.00	5. OTHER					
1.5.01.01	Meteorite Impact	– Cratering, host rock removal – Exhumation of waste – Alteration of flow pathways	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.5.01.02	Extraterrestrial Events	– Solar systems (supernova) – Celestial activity (sun - solar flares, gamma-ray bursters, moon - earth tides) – Alien life forms	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.5.03.01	Earth Planetary Changes	– Changes in earth's magnetic field – Changes in earth's gravitational field (tides) – Changes in ocean currents	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.0.00.00	2. DISPOSAL SYSTEM FACTORS					
2.1.00.00	1. WASTES AND ENGINEERED FEATURES					
2.1.01.00	1.01. INVENTORY					
2.1.01.01	Waste Inventory – Radionuclides – Nonradionuclides	– Composition – Enrichment / Burn-up	Yes	The species in the waste inventory are defined in *Materials > Species*. Thirty-five radionuclides and one nonradionuclide are included. The *RN_Inventory* component contains the data and calculations related to the three types of waste forms: *UNF_Inventory* for commercial UNF, *DOEHLW_Inventory* for existing DHLW, and *RWHLW_Inventory* for CHLW. The isotopic inventory of the commercial UNF is assumed to be represented by the PWR fuel with a burn-up of 60 GWd/MTIHM and 4.73% enrichment and aged 30 yr after discharge from reactor. The hypothetical CHLW is based on 99% removal of U and Pu from the commercial UNF inventory.	Yes	36 radionuclides are defined in the container :\Materials. Half-lives are defined for each radionuclide and several daughters are identified. The model accounts for the in-growth of daughters and isotopic mixing among radionuclides. The container at :\Container1\ RN_Inventory component contains the data and calculations related to the three types of waste forms : UNF_Inventory for commercial UNF, DOEHLW_Inventory for existing DHLW, and RWHLW_Inventory for CHLW. The isotopic inventory of the commercial UNF is assumed to be represented by the PWR fuel with a burn-up of 60 GWd/MTIHM and 4.73% enrichment and aged 30 yr after discharge from reactor.
2.1.01.02	Radioactive Decay and Ingrowth	– Decay chains – Decay products – Neutron activation	Yes	*Materials > Species* contains information about 36 species including the half-lives, activities, and daughter products and associated properties. The amounts of different species are contained in *RN_Inventory.*	Yes	The container at :\Materials includes information about 36 species including the half-lives, activities, and daughter products and associated properties. The amounts of different species are contained in :\Container1*RN_Inventory*. Decay and ingrowth for the Far Field are included in the FEHM DLL. The FEHM DLL is implemented at \Container1\Far_Field\FEHM_localize.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.01.03	Heterogeneity of Waste Inventory – Waste Package Scale – Repository Scale	– Composition – Enrichment / Burn-up – Damaged Area	Partially	The reference case includes three different waste types and their inventories. The UNF waste considers just one combination of enrichment and burn-up. The model does not specifically consider the waste form damaged area effect.	Yes	Waste package scale is specified in :\Container1\near_field_new\In_Package_volume\WP_configuration, and repository scale is specified in :\Container1\near_field_new\Repository_config. The container at :\Container1\RN_Inventory component contains the data and calculations related to the three types of waste forms: UNF_Inventory for commercial UNF, DOEHLW_Inventory for existing DHLW, and RWHLW_Inventory for CHLW. The isotopic inventory of the commercial UNF is assumed to be represented by the PWR fuel with a burn-up of 60 GWd/MTIHM and 4.73% enrichment and aged 30 yr after discharge from reactor.
2.1.01.04	Interactions Between Co-Located Waste		No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.02.00	1.02. WASTE FORM					
2.1.02.01	SNF (Commercial, DOE) Degradation – Alteration / Phase Separation – Dissolution / Leaching – Radionuclide Release	Degradation is dependent on: – Composition – Geometry / Structure – Enrichment / Burn-up – Surface Area – Gap and Grain Fraction – Damaged Area – THC Conditions [see also Mechanical Impact in 2.1.07.06 and Thermal-Mechanical Effects in 2.1.11.06]	Partially	UNF degradation is modeled in the container *UNF_WF* within the container *Waste_form_degradation*. The waste form degradation in the source-term analysis is modeled with the yearly fractional degradation rates (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates in the GDS conditions. All GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. In the current GDS model, for a given realization, a sampled constant rate is applied to all waste of the type being modeled; no temperature dependence is modeled at this time. In the model user chooses the waste inventory case for the simulation: Case 1: UNF + DHLW, and Case 2: DHLW + CHLW. The following are not included: geometry/structure, surface area effect, gap and GB fraction, damaged area, and TH conditions.	Partially	The waste form degradation in the source-term analysis is modeled with the yearly fractional degradation rates (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates in the GDS conditions. All GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. In the current GDS model a constant rate is applied to all waste; no temperature dependence is modeled at this time. (from 2010 GDSE Progress Report) This is implemented in the model at \Container1\near_field_new\Waste_form_degradation. Two types of waste form degradation rates are considered in the model: commercial UNF degradation rate (for UNF) and borosilicate glass waste form degradation rate (for DHLW and CHLW).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.02.02	HLW (Glass, Ceramic, Metal) Degradation – Alteration / Phase Separation – Dissolution / Leaching – Cracking – Radionuclide Release	Degradation is dependent on: – Composition – Geometry / Structure – Surface Area – Damaged / Cracked Area – Mechanical Impact – THC Conditions [see also Mechanical Impact in 2.1.07.07 and Thermal-Mechanical Effects in 2.1.11.06]	Partially	The waste form degradation in the source-term analysis is modeled with the yearly fractional degradation rates (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates in the GDS conditions. All GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. In the current GDS model, for a given realization, a sampled constant rate is applied to all waste of the type being modeled; no temperature dependence is modeled at this time. In the model user chooses the waste inventory case for the simulation: Case 1: UNF + DHLW, and Case 2: DHLW + CHLW. The following are not included: geometry/structure, surface area effect, damaged area, and TH conditions.	Partially	The waste form degradation in the source-term analysis is modeled with the yearly fractional degradation rates (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates in the GDS conditions. All GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. In the current GDS model a constant rate is applied to all waste; no temperature dependence is modeled at this time (from 2010 GDSE Progress Report). This implemented in the model at \Container1\near_field_new\Waste_form_degradation. Two types of waste form degradation rates are considered in the model: commercial UNF degradation rate (for UNF) and borosilicate glass waste form degradation rate (for DHLW and CHLW).
2.1.02.03	Degradation of Organic/Cellulosic Materials in Waste	[see also Complexation in EBS in 2.1.09.54]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.02.04	HLW (Glass, Ceramic, Metal) Recrystallization		No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.02.05	Pyrophoricity or Flammable Gas from SNF or HLW	[see also Gas Explosions in EBS in 2.1.12.04]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.02.06	SNF Cladding Degradation and Failure	– Initial damage – General Corrosion – Microbially Influenced Corrosion – Localized Corrosion – Enhanced Corrosion (silica, fluoride) – Stress Corrosion Cracking – Hydride Cracking – Unzipping – Creep – Internal Pressure – Mechanical Impact	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.03.00	1.03. WASTE CONTAINER					
2.1.03.01	Early Failure of Waste Packages	– Manufacturing defects – Improper sealing [see also Deviations from Design in 1.1.08.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.03.02	General Corrosion of Waste Packages	– Dry-air oxidation – Humid-air corrosion – Aqueous phase corrosion – Passive film formation and stability	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.03.03	Stress Corrosion Cracking (SCC) of Waste Packages	– Crack initiation, growth and propagation – Stress distribution around cracks	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.03.04	Localized Corrosion of Waste Packages	– Pitting – Crevice corrosion – Salt deliquescence [see also 2.1.09.06 Chemical Interaction with Backfill]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.03.05	Hydride Cracking of Waste Packages	– Hydrogen diffusion through metal matrix – Crack initiation and growth in metal hydride phases	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.03.06	Microbially Influenced Corrosion (MIC) of Waste Packages		No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.03.07	Internal Corrosion of Waste Packages Prior to Breach		No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.03.08	Evolution of Flow Pathways in Waste Packages	– Evolution of physical form of waste package – Plugging of cracks in waste packages [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Mechanical Impacts in 2.1.07.05, 2.1.07.06, and 2.1.07.07, Thermal-Mechanical Effects in 2.1.11.06 and 2.1.11.07]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.04.00	1.04. BUFFER / BACKFILL					
2.1.04.01	Evolution and Degradation of Backfill	– Alteration – Thermal expansion / Degradation – Swelling/Compaction – Erosion/Dissolution – Evolution of backfill flow pathways [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Mechanical Impact in 2.1.07.04, Thermal-Mechanical Effects in 2.1.11.08, Chemical Interaction in 2.1.09.06]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	The granite GDS model incorporates bentonite buffer, but does not include evolution or degradation of the buffer.
2.1.05.00	1.05. SEALS					
2.1.05.01	Degradation of Seals	– Alteration / Degradation / Cracking – Erosion / Dissolution [see also Mechanical Impact in 2.1.07.08, Thermal-Mechanical Effects in 2.1.11.09, Chemical Interaction in 2.1.09.08]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.06.00	1.06. OTHER EBS MATERIALS					
2.1.06.01	Degradation of Liner / Rock Reinforcement Materials in EBS	– Alteration / Degradation / Cracking – Corrosion – Erosion / Dissolution / Spalling [see also Mechanical Impact in 2.1.07.08, Thermal-Mechanical Effects in 2.1.11.09, Chemical Interaction in 2.1.09.07]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.00	1.07. MECHANICAL PROCESSES					
2.1.07.01	Rockfall	– Dynamic loading (block size and velocity) [see also Mechanical Effects on Host Rock in 2.2.07.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.02	– Drift Collapse	– Static loading (rubble volume) – Alteration of seepage – Alteration of EBS flow pathways – Alteration of EBS thermal environment [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Chemical Effects of Drift Collapse in 2.1.09.12, and Effects of Drift Collapse on TH in 2.1.11.04, Mechanical Effects on Host Rock in 2.2.07.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.07.03	Mechanical Effects of Backfill	– Protection of other EBS components from rockfall / drift collapse	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	The granite GDS model incorporates bentonite buffer, but does not include evolution or mechanical effects of the buffer.
2.1.07.04	Mechanical Impact on Backfill	– Rockfall / Drift collapse – Hydrostatic pressure – Internal gas pressure [see also Degradation of Backfill in 2.1.04.01 and Thermal-Mechanical Effects in 2.1.11.08]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	The granite GDS model incorporates bentonite buffer, but does not include evolution or mechanical impact on the buffer.
2.1.07.05	Mechanical Impact on Waste Packages	– Rockfall / Drift collapse – Waste package movement – Hydrostatic pressure – Internal gas pressure – Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.07]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.06	Mechanical Impact on SNF Waste Form	– Drift collapse – Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.06]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.07	Mechanical Impact on HLW Waste Form	– Drift collapse – Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.06]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.07.08	Mechanical Impact on Other EBS Components – Seals – Liner/Rock Reinforcement Materials – Waste Package Support Materials	– Rockfall / Drift collapse – Movement – Hydrostatic pressure – Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.09]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.09	Mechanical Effects at EBS Component Interfaces	– Component-to-component contact (static or dynamic)	Partially	The model includes creep deformation of salt rock, consolidation of crushed salt backfill around waste package, and closure of waste emplacement area. Repository brine flow analysis includes effect of the creep deformation and closure of the waste emplacement area.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.10	Mechanical Degradation of EBS	– Floor buckling – Fault displacement – Initial damage from excavation / construction – Consolidation of EBS components – Degradation of waste package support structure – Alteration of EBS flow pathways [see also Mechanical Effects from Preclosure in 1.1.02.02, Evolution of Flow Pathways in EBS in 2.1.08.06, Drift Collapse in 2.1.07.02, Degradation in 2.1.04.01, 2.1.05.01, and 2.1.06.01, and Mechanical Effects on Host Rock in 2.2.07.01]	Partially	The model includes creep deformation of salt rock, consolidation of crushed salt backfill around waste package, and closure of waste emplacement area. Repository brine flow analysis includes effect of the creep deformation and closure of the waste emplacement area.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.08.00	1.08. HYDROLOGIC PROCESSES					
2.1.08.01	Flow Through the EBS	– Saturated / Unsaturated flow – Preferential flow pathways – Density effects on flow – Initial hydrologic conditions – Flow pathways out of EBS [see also Open Boreholes in 1.1.01.01, Thermal-Hydrologic Effects from Preclosure in 1.1.02.03, Flow in Waste Packages in 2.1.08.02, Flow in Backfill in 2.1.08.03, Flow through Seals 2.1.08.04, Flow through Liner in 2.1.08.05, Thermal Effects on Flow in 2.1.11.10, Effects of Gas on Flow in 2.1.12.02]	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Hydrologic processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM. The repository brine flow abstractions are based on detailed process-level analysis of brine hydrologic processes in the consolidated closed waste disposal area.	No	A simplified representation of the EBS is used. Flow is not modeled in the EBS. The bentonite buffer is assumed to be saturated, but only diffusive transport is modeled.
2.1.08.02	Flow In and Through Waste Packages	– Saturated / Unsaturated flow – Movement as thin films or droplets	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Hydrologic processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM. The repository brine flow abstractions are based on detailed process-level analysis of brine hydrologic processes in the consolidated closed waste disposal area.	No	Waste Packages are assumed to degrade immediately in the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.08.03	Flow in Backfill	– Fracture / Matrix flow	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Hydrologic processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM. The repository brine flow abstractions are based on detailed process-level analysis of brine hydrologic processes in the consolidated closed waste disposal area. The analysis includes matrix flow only.	No	A simplified representation of the EBS is used. Flow is not modeled in the EBS. The bentonite buffer is assumed to be saturated, but only diffusive transport is modeled.
2.1.08.04	Flow Through Seals	– Fracture / Matrix flow	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Hydrologic processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	A simplified representation of the EBS is used. Flow is not modeled in the EBS. The bentonite buffer is assumed to be saturated, but only diffusive transport is modeled.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.08.05	Flow Through Liner / Rock Reinforcement Materials in EBS		No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Hydrologic processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	A simplified representation of the EBS is used. Flow is not modeled in the EBS. The bentonite buffer is assumed to be saturated, but only diffusive transport is modeled.
2.1.08.06	Alteration and Evolution of EBS Flow Pathways	– Drift collapse – Degradation/consolidation of EBS components – Plugging of flow pathways – Formation of corrosion products – Water ponding [see also Evolution of Flow Pathways in WPs in 2.1.03.08, Evolution of Backfill in 2.1.04.01, Drift Collapse in 2.1.07.02, and Mechanical Degradation of EBS in 2.1.07.10]	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Hydrologic processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM. The repository brine flow abstractions are based on detailed process-level analysis of brine hydrologic processes in the consolidated closed waste disposal area.	No	A simplified representation of the EBS is used. Flow is not modeled in the EBS. The bentonite buffer is assumed to be saturated, but only diffusive transport is modeled.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.08.07	Condensation Forms in Repository – On Tunnel Roof/Walls – On EBS Components	– Heat transfer (spatial and temporal distribution of temperature and relative humidity) – Dripping – Moisture movement [see also Heat Generation in EBS in 2.1.11.01, Effects on EBS Thermal Environment in 2.1.11.03 and 2.1.11.04]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Hydrologic processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	The current model assumes ambient temperatures.
2.1.08.08	Capillary Effects in EBS	– Wicking – Capillary barrier – Osmotic binding	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Hydrologic processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	A simplified representation of the EBS is used. Flow is not modeled in the EBS. The bentonite buffer is assumed to be saturated, but only diffusive transport is modeled.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.08.09	Influx/Seepage Into the EBS	– Water influx rate (spatial and temporal distribution) [see also Open Boreholes in 1.1.01.01, Thermal Effects on Flow in EBS in 2.1.11.10, Flow Through Host Rock in 2.2.08.01, Effects of Excavation on Flow in 2.2.08.04]	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Hydrologic processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM. The repository brine flow abstractions are based on detailed process-level analysis of brine hydrologic processes in the consolidated closed waste disposal area. The analysis includes brine flows into the waste disposal area by pressure gradients.	No	A simplified representation of the EBS is used. Flow is not modeled in the EBS. The bentonite buffer is assumed to be saturated, but only diffusive transport is modeled.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.00	1.09. CHEMICAL PROCESSES - CHEMISTRY					
2.1.09.01	Chemistry of Water Flowing into the Repository	– Chemistry of influent water (spatial and temporal distribution) [See also Chemistry in Host Rock 2.2.09.01]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	Partially	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. Different solubilities are specified for radionuclides at near field and at near- / far-field interface (:\Uncertain_Parameters\RN_Solubility). Radionuclides sorption coefficients are specified for bentonite buffer and granite host rock (:\Container1\near_field_new\Waste_form_degradation\Kd_bentonite, :\container_inputdat\stochastic_input_for_fehm).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.02	Chemical Characteristics of Water in Waste Packages	– Water composition (radionuclides, dissolved species, …) – Initial void chemistry (air / gas) – Water chemistry (pH, ionic strength, pCO2, …) – Reduction-oxidation potential – Reaction kinetics – Influent chemistry (from tunnels and/or backfill) [see also Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04] – Evolution of water chemistry / interaction with waste packages	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. Different solubilities are specified for radionuclides at near field and at near- / far-field interface (:\Uncertain_Parameters\RN_Solubility). Radionuclides sorption coefficients are specified for bentonite buffer and granite host rock (:\Container1\near_field_new\Waste_form_degradation\Kd_bentonite, :\container_inputdat\stochastic_input_for_fehm).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.03	Chemical Characteristics of Water in Backfill	– Water composition (radionuclides, dissolved species, …) – Water chemistry (pH, ionic strength, pCO2, …) – Reduction-oxidation potential – Reaction kinetics – Influent chemistry (from tunnels and/or waste packages) [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Tunnels in 2.1.09.04] – Evolution of water chemistry / interaction with backfill	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. Different solubilities are specified for radionuclides at near field and at near- / far-field interface (:\Uncertain_Parameters\RN_Solubility). Radionuclides sorption coefficients are specified for bentonite buffer and granite host rock (:\Container1\near_field_new\Waste_form_degradation\Kd_bentonite, :\container_inputdat\stochastic_input_for_fehm).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.04	Chemical Characteristics of Water in Tunnels	– Water composition (radionuclides, dissolved species, …) – Water chemistry (pH, ionic strength, pCO2, …) – Reduction-oxidation potential – Reaction kinetics – Influent chemistry (from construction / emplacement) – Initial chemistry (from construction/emplacement) [see also Chemical Effects from Preclosure in 1.1.02.01, Chemistry of Water Flowing in 2.1.09.01, Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03] – Evolution of water chemistry / interaction with seals, liner/rock reinforcement materials, waste package support materials	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. Different solubilities are specified for radionuclides at near field and at near- / far-field interface (:\Uncertain_Parameters\RN_Solubility). Radionuclides sorption coefficients are specified for bentonite buffer and granite host rock (:\Container1\near_field_new\Waste_form_degradation\Kd_bentonite, :\container_inputdat\stochastic_input_for_fehm).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.05	Chemical Interaction of Water with Corrosion Products – In Waste Packages – In Backfill – In Tunnels	– Corrosion product formation and composition (waste form, waste package internals, waste package) – Evolution of water chemistry in waste packages, in backfill, and in tunnels [contributes to Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. Different solubilities are specified for radionuclides at near field and at near- / far-field interface (:\Uncertain_Parameters\RN_Solubility). Radionuclides sorption coefficients are specified for bentonite buffer and granite host rock (:\Container1\near_field_new\Waste_form_degradation\Kd_bentonite, :\container_inputdat\stochastic_input_for_fehm).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.06	Chemical Interaction of Water with Backfill – On Waste Packages – In Backfill – In Tunnels	– Backfill composition and evolution (bentonite, crushed rock, ...) – Evolution of water chemistry in backfill and in tunnels – Enhanced degradation of waste packages (crevice corrosion) [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04, Localized Corrosion of WPs in 2.1.03.04]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	Partially	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. Different solubilities are specified for radionuclides at near field and at near- / far-field interface (:\Uncertain_Parameters\RN_Solubility). Radionuclides sorption coefficients are specified for bentonite buffer and granite host rock (:\Container1\near_field_new\Waste_form_degradation\Kd_bentonite, :\container_inputdat\stochastic_input_for_fehm).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.07	Chemical Interaction of Water with Liner / Rock Reinforcement and Cementitious Materials in EBS – In Backfill – In Tunnels	– Liner composition and evolution (concrete, metal, ...) – Rock reinforcement material composition and evolution (grout, rock bolts, mesh, ….) – Other cementitious materials composition and evolution – Evolution of water chemistry in backfill, and in tunnels [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	Partially	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. Different solubilities are specified for radionuclides at near field and at near- / far-field interface (:\Uncertain_Parameters\RN_Solubility). Radionuclides sorption coefficients are specified for bentonite buffer and granite host rock (:\Container1\near_field_new\Waste_form_degradation\Kd_bentonite, :\container_inputdat\stochastic_input_for_fehm).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.08	Chemical Interaction of Water with Other EBS Components – In Waste Packages – In Tunnels	– Seals composition and evolution – Waste Package Support composition and evolution (concrete, metal, …) – Other EBS components (other metals - Copper, …) – Evolution of water chemistry in backfill and in tunnels [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. Different solubilities are specified for radionuclides at near field and at near- / far-field interface (:\Uncertain_Parameters\RN_Solubility). Radionuclides sorption coefficients are specified for bentonite buffer and granite host rock (:\Container1\near_field_new\Waste_form_degradation\Kd_bentonite, :\container_inputdat\stochastic_input_for_fehm).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.09	Chemical Effects at EBS Component Interfaces	– Component-to-component contact (chemical reactions) – Consolidation of EBS components	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.10	Chemical Effects of Waste-Rock Contact	– Waste-to-host rock contact (chemical reactions) – Component-to-host rock contact (chemical reactions)	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.11	Electrochemical Effects in EBS	– Enhanced metal corrosion	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.12	Chemical Effects of Drift Collapse	– Evolution of water chemistry in backfill and in tunnels (from altered seepage, from altered thermal-hydrology) [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.13	Radionuclide Speciation and Solubility in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Dissolved concentration limits – Limited dissolution due to inclusion in secondary phase – Enhanced dissolution due to alpha recoil [controlled by Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). A module with improved treatment of the EBS is being developed for eventual use in the GPAM. Chemical processes within the EBS are not explicitly modeled. However, all GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. The radionuclide solubility analysis and abstraction is based on two different redox conditions representing chemically reducing and less reducing/slightly oxidizing conditions. The radionuclide solubility for reducing condition is applied to the near-field brines, and the solubility for less reducing/slightly oxidizing condition is applied to the interface and far-field waters.	Partially	Solubility limits in the bentonite are defined at \Uncertain_Parameters\RN_Solubility. Some radionuclides are modeled with unlimited solubility. The solubility limits are implemented at \Container1\near_field_new\Waste_form_degradation. The other features identified in this FEP are not considered in the transport calculations.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.50	1.09. CHEMICAL PROCESSES - TRANSPORT					
2.1.09.51	Advection of Dissolved Radionuclides in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Flow pathways and velocity – Advective properties (porosity, tortuosity) – Dispersion – Saturation [see also Gas Phase Transport in 2.1.12.03]	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM. The repository brine flow abstractions are based on detailed process-level analysis of brine hydrologic processes in the consolidated closed waste disposal area. The analysis includes brine inflows into and outflows out of the waste disposal area by pressure gradients.	No	Only diffusive transport is modeled in the EBS.
2.1.09.52	Diffusion of Dissolved Radionuclides in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Gradients (concentration, chemical potential) – Diffusive properties (diffusion coefficients) – Flow pathways and velocity – Saturation	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	Partially	Diffusive transport through the bentonite is modeled using the cell network at \Container1\near_field_new\Waste_form_degradation\UNF_WF\UNF_1diffWP_release, for UNF and at \Container1\near_field_new\Waste_form_degradation\HLW_Glass_WF\HLW_1diffWP_release for HLW Glass. The waste form is modeled using a fractional degradation rate that provides a source term for diffusive transport through the bentonite buffer. The waste package and tunnel are not considered in the calculations.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.53	Sorption of Dissolved Radionuclides in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Surface complexation properties – Flow pathways and velocity – Saturation [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	Partially	Sorption on the bentonite buffer material is modeled at \Container1\near_field_new\Waste_form_degradation. Some radionuclides are modeled with sorption coefficients of zero. Sorption coefficients are set to zero for all radionuclides for the degraded waste form. Sorption is not modeled on the waste package or in the tunnel.
2.1.09.54	Complexation in EBS	– Formation of organic complexants (humates, fulvates, organic waste) – Enhanced transport of radionuclides associated with organic complexants [see also Degradation of Organics in Waste in 2.1.02.03; see Radionuclide Speciation in 2.1.09.13 for inorganic complexation]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.55	Formation of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Formation of intrinsic colloids – Formation of pseudo colloids (host rock fragments, waste form fragments, corrosion products, microbes) – Formation of co-precipitated colloids – Sorption/attachment of radionuclides to colloids (clay, silica, waste form, FeOx, microbes)	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Colloids are not included in the model.
2.1.09.56	Stability of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Chemical stability of attachment (dependent on water chemistry) – Mechanical stability of colloid (dependent on colloid size, gravitational setting)	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Colloids are not included in the model. This may be considered for inclusion in a sensitivity study of glaciation impact.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.57	Advection of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Flow pathways and velocity – Advective properties (porosity, tortuosity) – Dispersion – Saturation – Colloid concentration	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Colloids are not included in the model.
2.1.09.58	Diffusion of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Gradients (concentration, chemical potential) – Diffusive properties (diffusion coefficients) – Flow pathways and velocity – Saturation – Colloid concentration	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Colloids are not included in the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.59	Sorption of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Surface complexation properties – Flow pathways and velocity – Saturation – Colloid concentration [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Colloids are not included in the model.
2.1.09.60	Sorption of Colloids at Air-Water Interface in EBS		No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Colloids are not included in the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.61	Filtration of Colloids in EBS	– Physical filtration or trapping (dependent on flow pathways, colloid size) – Electrostatic filtration	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Colloids are not included in the model.
2.1.09.62	Radionuclide Transport Through Liners and Seals	– Advection – Dispersion – Diffusion – Sorption [contributes to Radionuclide release from EBS in 2.1.09.63]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	The model currently does not include liners or seals.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.63	Radionuclide Release from the EBS – Dissolved – Colloidal – Gas Phase	– Spatial and temporal distribution of releases to the host rock (due to varying flow pathways and velocities, varying component degradation rates, varying transport properties) [contributions from Dissolved in 2.1.09.51/52/53, Colloidal in 2.1.09.57/58/59, Gas Phase in 2.1.12.03, Liners and Seals in 2.1.09.62]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells).Transport processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	Partially	Mass release from the EBS is collected at \Container1\near_field_new\WF_RN_release\WF_RN_Release_Case1. The mass flux of individual radionuclides is calculated as a function of time. Colloids are not included in the model. Gas Phase Transport is not included in the model.
2.1.10.00	1.10. BIOLOGICAL PROCESSES					
2.1.10.01	Microbial Activity in EBS – Natural – Anthropogenic	– Effects on corrosion – Formation of complexants – Formation of microbial colloids – Formation of biofilms – Biodegradation – Biomass production – Bioaccumulation [see also Microbially Influenced Corrosion in 2.1.03.06, Complexation in EBS in 2.1.09.54, Radiological Mutation of Microbes in 2.1.13.03]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Biological processes within the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Microbial activity is not modeled in the EBS.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.11.00	1.11. THERMAL PROCESSES					
2.1.11.01	Heat Generation in EBS	– Heat transfer (spatial and temporal distribution of temperature and relative humidity) [see also Thermal-Hydrologic Effects from Preclosure in 1.1.02.03, Waste Inventory in 2.1.01.01]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.
2.1.11.02	Exothermic Reactions in EBS	– Oxidation of SNF – Hydration of concrete	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.11.03	Effects of Backfill on EBS Thermal Environment	– Thermal blanket – Condensation	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.
2.1.11.04	Effects of Drift Collapse on EBS Thermal Environment	– Thermal blanket – Condensation	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.11.05	Effects of Influx (Seepage) on Thermal Environment	– Temperature and relative humidity (spatial and temporal distribution) [see also Influx/Seepage into EBS in 2.1.08.09]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.
2.1.11.06	Thermal-Mechanical Effects on Waste Form and In-Package EBS Components	– Alteration – Cracking – Thermal expansion / stress	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.11.07	Thermal-Mechanical Effects on Waste Packages	– Thermal sensitization / phase changes – Cracking – Thermal expansion / stress/ creep	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.
2.1.11.08	Thermal-Mechanical Effects on Backfill	– Alteration – Cracking – Thermal expansion / stress	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM. The repository brine flow analysis includes creep deformation and consolidation of crushed salt backfill in the waste disposal area, and associated brine flows through the consolidated backfill.	No	Thermal effects will be added in a future revision of the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.11.09	Thermal-Mechanical Effects on Other EBS Components – Seals – Liner / Rock Reinforcement Materials – Waste Package Support Structure	– Alteration – Cracking – Thermal expansion / stress	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.
2.1.11.10	Thermal Effects on Flow in EBS	– Altered influx/seepage – Altered saturation / relative humidity (dry-out, resaturation) – Condensation	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.11.11	Thermally-Driven Flow (Convection) in EBS	– Convection	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.
2.1.11.12	Thermally-Driven Buoyant Flow / Heat Pipes in EBS	– Vapor flow	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.11.13	Thermal Effects on Chemistry and Microbial Activity in EBS		No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.
2.1.11.14	Thermal Effects on Transport in EBS	– Thermal diffusion (Soret effect) – Thermal osmosis	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Thermal effects will be added in a future revision of the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.12.00	1.12. GAS SOURCES AND EFFECTS					
2.1.12.01	Gas Generation in EBS	– Repository Pressurization – Mechanical Damage to EBS Components – He generation from waste from alpha decay – H_2 generation from waste package corrosion – CO_2, CH_4, and H_2S generation from microbial degradation – Vaporization of water	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Gas generation and its effects in the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM. The repository brine flow abstractions are based on detailed process-level analysis of brine hydrologic processes in the consolidated closed waste disposal area. The analysis includes brine inflows into and outflows out of the waste disposal area by pressure gradients due to lithostatic pressure away from the disposal area and pressurization of waste disposal area from corrosion gas generation and creep closure.	No	Gas generation and its effect on the EBS are not included in the model.
2.1.12.02	Effects of Gas on Flow Through the EBS	– Two-phase flow – Gas bubbles [see also Buoyant Flow/Heat Pipes in 2.1.11.12]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Gas generation and its effects in the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Gas generation and its effect on the EBS are not included in the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.12.03	Gas Transport in EBS	– Gas phase transport – Gas phase release from EBS	Partially	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Gas generation and its effects in the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM. The repository brine flow abstractions are based on detailed process-level analysis of brine hydrologic processes in the consolidated closed waste disposal area. The analysis includes brine inflows into and outflows out of the waste disposal area by pressure gradients due to lithostatic pressure away from the disposal area and pressurization of waste disposal area from corrosion gas generation and creep closure.	No	Gas generation and its effect on the EBS are not included in the model.
2.1.12.04	Gas Explosions in EBS	[see also Flammable Gas from Waste in 2.1.02.05]	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Gas generation and its effects in the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	Gas generation and its effect on the EBS are not included in the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.13.00	1.13. RADIATION EFFECTS					
2.1.13.01	Radiolysis – In Waste Package – In Backfill – In Tunnel	– Gas generation – Altered water chemistry	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Radiation effects in the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	The effects of radiolysis are not included in the model.
2.1.13.02	Radiation Damage to EBS Components – Waste Form – Waste Package – Backfill – Other EBS Components	– Enhanced waste form degradation – Enhanced waste package degradation – Enhanced backfill degradation – Enhanced degradation of other EBS components (liner/rock reinforcement materials, seals, waste support structure)	No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Radiation effects in the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	The effects of radiolysis are not included in the model.
2.1.13.03	Radiological Mutation of Microbes		No	The current salt GDS model considers the EBS in a very simplistic manner. Waste packages are assumed to fail immediately, and waste forms are given a fractional degradation rate that is used to calculate waste form radionuclide release into the near field. Flow starts at the five near-field mixing cells (Near_field > WF_RN_release > NF_MixingCells). Radiation effects in the EBS are not considered. A module with improved treatment of the EBS is being developed for eventual use in the GPAM.	No	The effects of radiolysis are not included in the model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.14.00	1.14. NUCLEAR CRITICALITY					
2.1.14.01	Criticality In-Package	– Formation of critical configuration	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.14.02	Criticality in EBS or Near-Field	– Formation of critical configuration	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.00.00	2. GEOLOGICAL ENVIRONMENT					
2.2.01.00	2.01. EXCAVATION DISTURBED ZONE (EDZ)					
2.2.01.01	Evolution of EDZ	– Lateral extent, heterogeneities – Physical properties – Flow pathways – Chemical characteristics of groundwater in EDZ – Radionuclide speciation and solubility in EDZ – Thermal-mechanical effects – Thermal-chemical alteration [see also Mechanical Effects of Excavation in 1.1.02.02]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	Partially	EDZ is modeled as a simple interface between near-field and far-field conditions. Radionuclide solubility is defined at \Uncertain_Parameters\RN_Solubility and they are implemented at \Container1\NF_Interface. Some radionuclides are assigned unlimited solubility. The other features and processes identified in this FEP are not currently modeled.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.02.00	2.02. HOST ROCK					
2.2.02.01	Stratigraphy and Properties of Host Rock	– Rock units – Thickness, lateral extent, heterogeneities, discontinuities, contacts – Physical properties – Flow pathways [see also Fractures in 2.2.05.01 and Faults in 2.2.05.02]	Partially	The salt bed that comprises the host rock is treated in a generic, stylized manner. See FEP 0.1.03.01 for location of dimensions of the various model domains. Heterogeneities and discontinuities are not considered. Flow in the rock above and through the EBS is not considered. Flow starts below the EBS at the five near-field mixing cells (cells and properties in Near_field > WF_RN_release). The properties of units in different model domains, including the repository and near field, are located in SaltGDSE_Parameters. The contact with the near-field marker bed is modeled using interface mixing cells (cells and properties in NF_Interface > IF_SaltBlock_Transport).	Partially	The physical dimensions of the repository area and the porosity of the host rock are implemented at \Container1\near_field_new\Repository_config\GDSE_NF_volume.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.03.00	2.03. OTHER GEOLOGIC UNITS					
2.2.03.01	Stratigraphy and Properties of Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	– Rock units – Thickness, lateral extent, heterogeneities, discontinuities, contacts – Physical properties – Flow pathways [see also Fractures in 2.2.05.01 and Faults in 2.2.05.02]	Partially	The non-host rock geologic units are treated in a generic, stylized manner. Processes in non-host rock above the EBS are not considered. A marker bed below the repository in the near field and far field provides the major pathway for radionuclide release and transport to the biosphere. This marker bed is assumed to be a mixture of evaporite minerals (such as anhydrite) and clay. It is 1-m thick and has the same width as the repository (see FEP 0.1.03.01 for location of dimensions of the various model domains). The properties of units in different model domains, including the near- and far-field marker bed, are located in SaltGDSE_Parameters. Heterogeneities and discontinuities are not considered. The contact with the near-field marker bed is modeled using interface rock mixing cells (cells and properties in NF_Interface > IF_SaltBlock_Transport). The near-field marker bed mixing cells and properties are located in NF_MB_Transport > NF_MB_Transport. The far-field marker bed mixing cells and properties are located in FFMB_Transport.	Yes	These features are defined in the FEHM DLL. The FEHM DLL is called at \Container1\Far_Field\FEHM_localize.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.05.00	2.05. FLOW AND TRANSPORT PATHWAYS					
2.2.05.01	Fractures – Host Rock – Other Geologic Units	– Rock properties [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	Partially	Fracture properties are included in the FEHM DLL for calculations in the Far Field. The properties are implemented at \container_inputdat. The conceptual model has radionuclides being transported from failed waste packages to the nearby aquifer through fast fracture flow. FEHM DLL simulates the radionuclides reactive transport through the fracture and matrix in the far field.
2.2.05.02	Fractures – Host Rock – Other Geologic Units	– Rock properties [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	Partially	Fractures are included in the FEHM DLL for calculations in the Far Field.
2.2.05.03	Alteration and Evolution of Geosphere Flow Pathways – Host Rock – Other Geologic Units	– Changes In rock properties – Changes in faults – Changes in fractures – Plugging of flow pathways – Changes in saturation [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01, Fractures in 2.2.05.01, and Faults in 2.2.05.02] [see also Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07]	Partially	The repository brine flow abstractions are based on detailed process-level analysis of brine hydrologic processes in the consolidated closed waste disposal area. The analysis includes brine inflows into and outflows out of the waste disposal area by pressure gradients due to lithostatic pressure away from the disposal area and pressurization of waste disposal area from corrosion gas generation and creep closure.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.07.00	2.07. MECHANICAL PROCESSES					
2.2.07.01	Mechanical Effects on Host Rock	– From subsidence – From salt creep – From clay deformation – From granite deformation (rockfall / drift collapse into tunnels – Chemical precipitation/ dissolution – Stress regimes [see also Subsidence in 1.2.02.01, Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.07.02	Mechanical Effects on Other Geologic Units	– From subsidence – Chemical precipitation / dissolution – Stress regimes [see also Subsidence in 1.2.02.01, Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.08.00	2.08. HYDROLOGIC PROCESSES					
2.2.08.01	Flow Through the Host Rock	– Saturated flow – Fracture flow / matrix imbibition – Unsaturated flow (fingering, capillarity, episodicity, perched water) – Preferential flow pathways – Density effects on flow – Flow pathways in Host Rock [see also Influx/Seepage into EBS in 2.1.08.09, Alteration of Flow Pathways in 2.2.05.03, Thermal Effects on Flow in 2.2.11.01, Effects of Gas on Flow in 2.2.12.02]	Partially	Flow above the repository is not considered. Flow starts below the EBS with five near-field mixing cells (cells and properties in Near_field > WF_RN_release). Mixing cells are used to provide a better representation of diffusive flow and transport, which appears to be the dominant flow and transport mechanism for very low brine flows (as seen in recent Bragflo analysis). However, both advective flow and diffusive flow are modeled. The contact with the near-field marker bed is modeled using interface rock mixing cells (cells and properties in NF_Interface > IF_SaltBlock_Transport). The first near-field cell flows (advective and diffusive) into the first interface cell, the second near-field cells flows into the second interface cell, the third near-field cell flows into the third interface cell, and so on. A similar pattern occurs in the connections between the interface cells and the five near-field marker bed cells (cells and properties in NF_MB_Transport > NF_MB_Transport). In addition, there is diffusive flow from cell 1 to 2 to 3 and so on within each set of five cells.	Partially	Fracture properties are included in the FEHM DLL for calculations in the Far Field. The properties are implemented at \container_inputdat. The conceptual model has radionuclides being transported from failed waste packages to the nearby aquifer through fast fracture flow. FEHM DLL simulates the radionuclides reactive transport through the fracture and matrix in the far field.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.08.02	Flow Through the Other Geologic Units – Confining units – Aquifers	– 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 [see also Alteration of Flow Pathways in 2.2.05.03, Thermal Effects on Flow in 2.2.11.01, Effects of Gas on Flow in 2.2.12.02]	No	Flow above the repository is not considered. Flow starts below the EBS with five near-field mixing cells (cells and properties in Near_field > WF_RN_release). Mixing cells are used to provide a better representation of diffusive flow and transport, which appears to be the dominant flow and transport mechanism for very low brine flows (as seen in recent Bragflo analysis). However, both advective flow and diffusive flow are modeled. The five near-field cells flow into five interface rock mixing cells (cells and properties in NF_Interface > IF_SaltBlock_Transport). The first near-field cell flows (advective and diffusive) into the first interface cell, the second near-field cells flows into the second interface cell, the third near-field cell flows into the third interface cell, and so on. A similar pattern occurs in the connections between the interface cells and the five near-field marker bed cells (cells and properties in NF_MB_Transport > NF_MB_Transport). In addition, there is diffusive flow from cell 1 to 2 to 3 and so on within each set of five cells. The five near-field marker bed cells are also connected to each other in series (advective and diffusive flow) with all flow going through the fifth cell. This fifth cell flows into the first of five far-field marker bed cells (FFMB_Transport). The five far-field marker bed cells are also connected in series ending with the fifth cell, which is connected to a far-field sink.	Partially	Saturated flow is implemented in the FEHM DLL, but the details are not visible in the GoldSim Model file. The FEHM DLL is called at \Container1\Far_Field\FEHM_localize. Fracture properties are included in the FEHM DLL for calculations in the Far Field. The properties are implemented at \container_inputdat. The conceptual model has radionuclides being transported from failed waste packages to the nearby aquifer through fast fracture flow. FEHM DLL simulates the radionuclides reactive transport through the fracture and matrix in the far field.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.08.03	Effects of Recharge on Geosphere Flow – Host Rock – Other Geologic Units	– Infiltration rate – Water table rise/decline [see also Infiltration 2.3.08.03]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.08.04	Effects of Repository Excavation on Flow Through the Host Rock	– Saturated flow (flow sink) – Unsaturated flow (capillary diversion, drift shadow) – Influx/Seepage into EBS (film flow, enhanced seepage [see also Influx/Seepage into EBS in 2.1.08.09]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.08.05	Condensation Forms in Host Rock	– Condensation cap – Shedding [see also Thermal Effects on Flow in Geosphere in 2.2.11.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.08.06	Flow Through EDZ	– Saturated / Unsaturated flow – Fracture / Matrix flow	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	Partially	Flow through the EDZ is modeled at \Container1\NF_Interface. Saturated flow is modeled. Unsaturated flow is not modeled. Fracture properties are not identified.
2.2.08.07	Mineralogic Dehydration	– Dehydration reactions release water and may lead to volume changes	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.08.08	Groundwater Discharge to Biosphere Boundary	– Surface discharge (water table, capillary rise, surface water) – Flow across regulatory boundary	Partially	The biosphere model used in the salt GDS model uses a dilution rate of 1E4 m3/yr in the aquifer from which a drinking water well withdraws water.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.08.09	Groundwater Discharge to Well	– Human use (drinking water, bathing water, industrial) – Agricultural use (irrigation, animal watering)	Partially	The biosphere model used in the salt GDS model uses a water consumption rate of 1.2 m3/yr for the exposed individual.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.00	2.09.CHEMICAL PROCESSES - CHEMISTRY					
2.2.09.01	Chemical Characteristics of Groundwater in Host Rock	– Water composition (radionuclides, dissolved species, …) – Water chemistry (temperature, pH, Eh, ionic strength …) – Reduction-oxidation potential – Reaction kinetics – Interaction with EBS – Interaction with host rock [see also Chemistry in Tunnels in 2.1.09.04, Chemical Interactions and Evolution in 2.2.09.03] [contributes to Chemistry of Water Flowing into Repository in 2.1.09.01]	Partially	The salt GDS model does not explicitly consider the chemical characteristics of the groundwater in the host rock. However, there is an expectation that the chemical processes in the geologic environment and the EBS will result in chemically reducing conditions in the EBS with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate of the waste forms is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. The radionuclide solubility in the far-field water is based on the water chemistry of dilute brine with slightly chemically oxidizing condition.	No	The granite GDS model does not explicitly consider the chemical characteristics of the groundwater in the host rock. However, there is an expectation that the chemical processes in the geologic environment and the EBS will result in chemically reducing conditions in the EBS with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate of the waste forms is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions. Different solubilities are specified for radionuclides at near field and at near-/ far-field interface (:\Uncertain_Parameters\RN_Solubility). Radionuclides sorption coefficients are specified for bentonite buffer and granite host rock (:\Container1\near_field_new\Waste_form_degradation\Kd_bentonite, :\container_inputdat\stochastic_input_for_fehm).

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.02	Chemical Characteristics of Groundwater in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Water composition (radionuclides, dissolved species, …) – Water chemistry (temperature, pH, Eh, ionic strength …) – Reduction-oxidation potential – Reaction kinetics - Interaction with other geologic units [see also Chemical Interactions and Evolution in 2.2.09.04]	No	The salt GDS model does not explicitly consider the chemical characteristics of groundwater in non-host-rock units. However, there is an expectation that the chemical processes in the geologic environment and the EBS will result in chemically reducing conditions in the EBS with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate of the waste forms is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	The granite GDS model does not explicitly consider the chemical characteristics of groundwater in non-host rock units.
2.2.09.03	Chemical Interactions and Evolution of Groundwater in Host Rock	– Host rock composition and evolution (granite, clay, salt ...) – Evolution of water chemistry in host rock – Chemical effects on density – Interaction with EBS – Reaction kinetics – Mineral dissolution/precipitation – Redissolution of precipitates after dry-out [contributes to Chemistry in Host Rock in 2.2.09.01]	No	The salt GDS model does not explicitly consider the chemical interactions and evolution of groundwater in the host rock. However, there is an expectation that the chemical processes in the geologic environment and the EBS will result in chemically reducing conditions in the EBS with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate of the waste forms is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.04	Chemical Interactions and Evolution of Groundwater in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Host rock composition and evolution (granite, clay, salt ...) – Evolution of water chemistry in host rock – Chemical effects on density – Reaction kinetics – Mineral dissolution/precipitation – Recharge chemistry [contributes to Chemistry in Other Geologic Units in 2.2.09.02]	No	The salt GDS model does not explicitly consider the chemical interactions and evolution of groundwater in non-host-rock units. However, there is an expectation that the chemical processes in the geologic environment and the EBS will result in chemically reducing conditions in the EBS with varying degrees of redox conditions of water in contact with the waste form. The fractional degradation rate of the waste forms is modeled with a distribution that captures the potential range of degradation rates in expected GDS conditions.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.05	Radionuclide Speciation and Solubility in Host Rock	– Dissolved concentration limits [controlled by Chemistry in Host Rock in 2.2.09.01]	Yes	The species in the waste inventory are defined in Materials > Species. Thirty-five radionuclides and one nonradionuclide are included. Various daughter products are also included. The solubility of the species in water is defined in Materials > Default_Solubility and Solubility_in_Water. The solubility in near-field water is located in SaltGDSE_Parameters > RN_Solubility > Solubility_NF_salt and Sol_NF_SaltBrine. Reducing conditions are assumed.	Yes	Solubility limits in the host rock are defined at \Uncertain_Parameters\RN_Solubility and implemented at \Container1\near_field_new\WF_RN_release\WF_RN_Release_Case1. Some radionuclides are modeled with unlimited solubility.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.06	Radionuclide Speciation and Solubility in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Dissolved concentration limits [controlled by Chemistry in Other Geologic Units in 2.2.09.02]	Yes	The species in the waste inventory are defined in Materials > Species. Thirty-five radionuclides and one nonradionuclide are included. Various daughter products are also included. The solubility of the species in water is defined in Materials > Default_Solubility and Solubility_in_Water. The solubility in near-field and far-field interface water is located in SaltGDSE_Parameters > RN_Solubility > Solubility_FF_salt and Sol_FF_SaltBrine. In general, reducing conditions are assumed; however, SaltGDSE_Parameters > RN_Solubility > Solubility_FF_salt > AddSol_Salt_LessReducing provides for conditions that are less reducing or slightly oxidizing (far-field slat brine).	Yes	Solubility limits in the EDZ and the Far Field are defined at \Uncertain_Parameters\RN_Solubility and are implemented for the near-far filed interface at \Container1\NF_Interface. Some radionuclides are modeled with unlimited solubility.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.50	2.09. CHEMICAL PROCESSES - TRANSPORT					
2.2.09.51	Advection of Dissolved Radionuclides in Host Rock	– Flow pathways and velocity – Advective properties (porosity, tortuosity) – Dispersion – Matrix diffusion – Saturation [see also Gas Phase Transport in 2.2.12.03]	Yes	The near-field flow and transport in the host rock are modeled using five mixing cells. The interface between the near-field host rock and the near-field marker bed is also modeled using five mixing cells. Both advective and diffusive fluxes are calculated (see FEP 2.2.08.01). The radionuclide release into the near-field mixing cells is calculated with the function Near_field > WF_RN_release > Total_WF_Release. Advective fluxes from the near-field mixing cells to the interface mixing cells are calculated in Near_field > WF_RN_release > AdvFlux_NF with the results contained in Results_NF_MixingCell. Advective fluxes from the interface cells are calculated in NF_Interface > IF_SaltBlock_Transport > AdvFlux_IFBlock with the results contained in NF_Interface > IF_SaltBlock_Results. Matrix diffusion is the only process not included. Full saturation is assumed for the entire simulation period.	Yes	The conceptual model has radionuclides being transported from failed waste packages to the nearby aquifer through fast fracture flow. FEHM DLL simulates the radionuclides reactive transport through the fracture and matrix in the far field with advection, matrix diffusion and sorption processes included.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.52	Advection of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Flow pathways and velocity – Advective properties (porosity, tortuosity) – Dispersion – Matrix diffusion – Saturation [see also Gas Phase Transport in 2.2.12.03]	Yes	The flow and transport in the marker beds are modeled using a total of ten mixing cells (five for near field and five for far field). Both advective and diffusive fluxes are calculated (see FEP 2.2.08.02). Advective fluxes from the interface mixing cells into the near-field marker bed cells are calculated in NF_Interface > IF_SaltBlock_Transport > AdvFlux_IFBlock with the results contained in NF_Interface > IF_SaltBlock_Results. The advective mass flux from the near-field marker bed (cell 5) to the far-field marker bed (cell 1) is contained in NF_MB_Transport > NF_MB_results > AdvMassFlux_NFMB. The advective mass flux from the far-field marker bed (cell 5) to the far-field sink is contained in FF_MB_Transport > FF_MB_results > AdvMAssFlux_FFMB. Matrix diffusion is the only process not included. Full saturation is assumed for the entire simulation period.	Yes	Advection of dissolved radionuclides is included in the FEHM DLL. The FEHM DLL is implemented at \Container1\Far_Field\FEHM_localize. The calculations completed using the FEHM DLL include advection, matrix diffusion, sorption and dispersion. Rock properties for the FEHM DLL are defined at \container_inputdat.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			**Capability Included in Salt GDS Model**		**Capability Included in Crystalline (Saturated Granite) GDS Model**	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.53	Diffusion of Dissolved Radionuclides in Host Rock	– Gradients (concentration, chemical potential) – Diffusive properties (diffusion coefficients) – Flow pathways and velocity – Saturation	Yes	The near-field flow and transport in the host rock are modeled using five mixing cells. The interface between the near-field host rock and the near-field marker bed is also modeled using five mixing cells. Both advective and diffusive fluxes are calculated (see FEP 2.2.08.01). The radionuclide release into the near-field mixing cells is calculated with the function Near_field > WF_RN_release > Total_WF_Release. Diffusive fluxes from the near-field mixing cells are calculated in Near_field > WF_RN_release > DiffFlux_NF with the results contained in Results_NF_MixingCell. Diffusive fluxes from the interface cells are calculated in NF_Interface > IF_SaltBlock_Transport > DiffFlux_IFBlock with the results contained in NF_Interface > IF_SaltBlock_Results. Full saturation is assumed for the entire simulation period.	Yes	Diffusion of dissolved radionuclide through the bentonite buffer is modeled using a cell network defined at \Container1\near_field_new\Waste_form_degradation\UNF_WF\UNF_1diffWP_release for UNF and defined at \Container1\near_field_new\Waste_form_degradation\HLW_Glass_WF\HLW_1diffWP_release for HLW glass. Diffusion of dissolved radionuclides in the far field is included in the FEHM DLL. The FEHM DLL is implemented at \Container1\Far_Field\FEHM_localize. The calculations completed using the FEHM DLL include advection, matrix diffusion, sorption and dispersion. Rock properties for the FEHM DLL are defined at \container_inputdat.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.54	Diffusion of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Gradients (concentration, chemical potential) – Diffusive properties (diffusion coefficients) – Flow pathways and velocity – Saturation	Yes	The flow and transport in the marker beds are modeled using a total of ten mixing cells (five for near field and five for far field). Both advective and diffusive fluxes are calculated (see FEP 2.2.08.02). Diffusive fluxes from the interface mixing cells into the near-field marker bed cells are calculated in NF_Interface > IF_SaltBlock_Transport > AdvFlux_IFBlock with the results contained in NF_Interface > IF_SaltBlock_Results. The advective mass flux from the near-field marker bed (cell 5) to the far-field marker bed (cell 1) is contained in NF_MB_Transport > NF_MB_results > DiffMassFlux_NFMB. The diffusive mass flux from the far-field marker bed (cell 5) to the far-field sink is contained in FF_MB_Transport > FF_MB_results > DiffMAssFlux_FFMB. Full saturation is assumed for the entire simulation period.	Yes	Matrix diffusion is included in the calculations done using the FEHM DLL.
2.2.09.55	Sorption of Dissolved Radionuclides in Host Rock	– Surface complexation properties – Flow pathways and velocity – Saturation [see also Chemistry in Host Rock in 2.2.09.01]	Partially	In the current version of the salt GDS model, there is no radionuclide sorption in the near-field host rock or the interface between the host rock and the near-field marker bed. The model includes sorption in the underlying interbed (reference case pathway) and overlying carbonate aquifer (human intrusion case pathway).	Yes	Sorption coefficients for bentonite are defined at \Container1\near_field_new\Waste_form_degradation\Kd_bentonite and are implemented at \Container1\near_field_new\Waste_form_degradation. Some radionuclides are modeled with sorption coefficients set equal to zero. Sorption is included in the calculations for far field done using the FEHM DLL

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.56	Sorption of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Surface complexation properties – Flow pathways and velocity – Saturation [see also Chemistry in Host Rock in 2.2.09.01]	Yes	The sorption coefficients (Kd's) for the near-field and far-field marker beds are found in SaltGDSE_Parameters > Salt_Transport > Salt_Kd.	Yes	Sorption coefficients for the Far Field are defined at \container_inputdat. These sorption coefficients are implemented in the FEHM DLL and the details of the implementation are not visible in GoldSim.
2.2.09.57	Complexation in Host Rock	– Presence of organic complexants (humates, fulvates, carbonates, …) – Enhanced transport of radionuclides associated with organic complexants [see Radionuclide Speciation in 2.2.09.05 for inorganic complexation]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.58	Complexation in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Presence of organic complexants (humates, fulvates, carbonates, …) – Enhanced transport of radionuclides associated with organic complexants [see Radionuclide Speciation in 2.2.09.06 for inorganic complexation]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.59	Colloidal Transport in Host Rock	– Flow pathways and velocity – Saturation – Advection – Dispersion – Diffusion – Sorption – Colloid concentration	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.60	Colloidal Transport in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Flow pathways and velocity – Saturation – Advection – Dispersion – Diffusion – Sorption – Colloid concentration	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.61	Radionuclide Transport Through EDZ	– Advection – Dispersion – Diffusion – Sorption	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	Partially	Advection through the EDZ is modeled using a mixing cell at \Container1\NF_Interface. Diffusive transport and sorption are not included in this part of the model.
2.2.09.62	Dilution of Radionuclides in Groundwater – Host Rock – Other Geologic Units	– Mixing with uncontaminated groundwater – Mixing at withdrawal well [see also Groundwater Discharge to Well in 2.2.08.09]	Partially	The biosphere model used in the salt GDS model uses a dilution rate of 1E4 m3/yr in the aquifer from which a drinking water well withdraws water.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.63	Dilution of Radionuclides with Stable Isotopes – Host Rock – Other Geologic Units	– Mixing with stable and/or naturally occurring isotopes of the same element	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.64	Radionuclide Release from Host Rock – Dissolved – Colloidal – Gas Phase	– 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) [contributions from Dissolved in 2.2.09.51/53/55, Colloidal in 2.2.09.59, Gas Phase in 2.2.12.03, EDZ in 2.2.09.61]	Partially	Dissolved radionuclides are released from the near-field mixing cells to the interface cells before going to the near-field marker bed cells (non-host rock). The mass fluxes from the near field are captured in Near_field > WF_RN_release > Results_NF_Mixing Cell. The mass fluxes from the interface are captured in NF_Interface > IF_SaltBlock_Results. Release through colloids or a gas phase is not included at this time.	Partially	Release of radionuclide mass from the host rock is implemented at \Container1\near_field_new\WF_RN_release\WF_RN_Release_Case1. Mass flux of individual radionuclides as a function of time is calculated. Radionuclide transport by colloids or by gas phase transport is not included.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.65	Radionuclide Release from Other Geologic Units – Dissolved – Colloidal – Gas Phase	– Spatial and temporal distribution of releases to the Biosphere (due to varying flow pathways and velocities, varying transport properties) [see also Groundwater Discharge to Biosphere Boundary in 2.2.08.08, Groundwater Discharge to Well in 2.2.08.09, Recycling of Accumulated Radionuclides in 2.3.09.55] [contributions from Dissolved in 2.2.09.52/54/56, Colloidal in 2.2.09.60, Gas Phase in 2.2.12.03]	Partially	Dissolved radionuclides are released from the last far-field mixing cell to the biosphere. The mass flux from the far-field marker bed is calculated with the function FF_MB_Transport > MassFlux_FF_MB, which is then used in the biosphere calculations. Release through colloids or a gas phase is not included at this time.	Partially	Release of radionuclide mass from the Far Field is implemented at \Container1\Far_Field\sink. Mass flux of individual radionuclides as a function of time is calculated as output from the FEHM DLL. Radionuclide transport by colloids or be gas phase transport is not included.
2.2.10.00	2.10. BIOLOGICAL PROCESSES					
2.2.10.01	Microbial Activity in Host Rock	Formation of complexants – Formation and stability of microbial colloids – Biodegradation – Bioaccumulation [see also Complexation in Host Rock in 2.2.09.57]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.10.02	Microbial Activity in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	Formation of complexants – Formation and stability of microbial colloids – Biodegradation – Bioaccumulation [see also Complexation in Other Geologic Units in 2.2.09.58]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.11.00	2.11. THERMAL PROCESSES					
2.2.11.01	Thermal Effects on Flow in Geosphere – Repository-Induced – Natural Geothermal	– Altered saturation / relative humidity (dry-out, resaturation) – Altered gradients, density, and/or flow pathways – Vapor flow – Condensation	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.
2.2.11.02	Thermally-Driven Flow (Convection) in Geosphere	– Convection	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.
2.2.11.03	Thermally-Driven Buoyant Flow / Heat Pipes in Geosphere	– Vapor flow	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.
2.2.11.04	Thermal Effects on Chemistry and Microbial Activity in Geosphere	– Mineral precipitation / dissolution – Altered solubility [contributes to Chemistry in 2.2.09.01 and 2.2.09.02]	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.
2.2.11.05	Thermal Effects on Transport in Geosphere	– Thermal diffusion (Soret effect) – Thermal osmosis	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.
2.2.11.06	Thermal-Mechanical Effects on Geosphere	– Thermal expansion / compression – Altered properties of fractures, faults, rock matrix	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
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)	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.
2.2.12.00	2.12. GAS SOURCES AND EFFECTS					
2.2.12.01	Gas Generation in Geosphere	– Degassing (clathrates, deep gases) – Microbial degradation of organics – Vaporization of water	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
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 [see also Buoyant Flow/Heat Pipes in 2.2.11.03]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.12.03	Gas Transport in Geosphere	– Gas phase transport – Gas phase release from Geosphere	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.14.00	2.14. NUCLEAR CRITICALITY					
2.2.14.01	Criticality in Far-Field	– Formation of critical configuration	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.00.00	3. SURFACE ENVIRONMENT					
2.3.01.00	3.01. SURFACE CHARACTERISTICS					
2.3.01.01	Topography and Surface Morphology	– Recharge and discharge areas	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.3.02.01	Surficial Soil Type	– Physical and chemical attributes	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.04.01	Surface Water	– Lakes, rivers, springs – Dams, reservoirs, canals, pipelines – Coastal and marine features – Water management activities	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.05.01	Biosphere Characteristics	– Climate – Soils – Flora and fauna – Microbes – Evolution of biosphere (natural, anthropogenic – e.g., acid rain) [see also Climate Change in 1.3.01.01, Surficial Soil Type in 2.3.02.01, Microbial Activity in 2.3.10.01]	No	The biosphere analysis (see model container Results) does not consider the various possible characteristics of the biosphere system. Instead it is focuses on a simple system with a single exposure pathway. The analysis assumes that a drinking water well is drilled 5 km down gradient from the edge of the repository. This well penetrates an aquifer that has been contaminated by radionuclides released from the repository. The analysis uses dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B). This biosphere analysis is used for all of the GDS models to facilitate comparison of disposal environments. In reality, it is unlikely that groundwater drawn from a bedded salt formation would be potable with significant treatment, and that recharge in the marker beds would sustain withdrawal from the well over a long period of time.	Partially	The Biosphere is modeled using the IAEA's ERB 1B. ERB 1B is implemented at \Container1\Results\ERB1B_Biosphere_model.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.3.07.00	3.07. MECHANICAL PROCESSES					
2.3.07.01	Erosion	– Weathering – Denudation – Subsidence [see also Subsidence in 1.2.02.01, Periglacial Effects in 1.3.04.01, Glacial Effects in 1.3.05.01, Surface Runoff in 2.3.08.02, and Soil and Sediment Transport in 2.3.09.53]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.07.02	Deposition	– Weathering	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.07.03	Animal Intrusion into Repository		No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.08.00	3.08. HYDROLOGIC PROCESSES					
2.3.08.01	Precipitation	– Spatial and temporal distribution [see also Climate Change in 1.3.01.01] [contributes to Infiltration in 2.3.08.03]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.3.08.02	Surface Runoff and Evapotranspiration	– Runoff, impoundments, flooding, increased recharge – Evaporation – Condensation – Transpiration (root uptake) [see also Climate Change in 1.3.01.01, Erosion in 2.3.07.01] [contributes to Infiltration in 2.3.08.03]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.08.03	Infiltration and Recharge	– Spatial and temporal distribution – Effect on hydraulic gradient – Effect on water table elevation [see also Topography in 2.3.01.01, Surficial Soil Type in 2.3.02.01] [contributes to Effects of Recharge in 2.2.08.03]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.00	3.09. CHEMICAL PROCESSES - CHEMISTRY					
2.3.09.01	Chemical Characteristics of Soil and Surface Water	– Altered recharge chemistry (natural) – Altered recharge chemistry (anthropogenic – e.g., acid rain) [contributes to Chemical Evolution of Groundwater in 2.2.09.04]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.02	Radionuclide Speciation and Solubility in Biosphere	– Dissolved concentration limits	No	The current biosphere model does not consider radionuclide chemical speciation and solubility.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.3.09.03	Radionuclide Alteration in Biosphere	– Altered physical and chemical properties – Isotopic dilution	Partially	The biosphere analysis (see model container Results) is very simplistic. It uses dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B). Altered physical and chemical properties of radionuclides in the biosphere are not considered. However, the process of dilution is included. Results > ERB1B_Biosphere_model > ERB1B_dilution_rate is used to calculate the dose factor (Results > ERB1B_Biosphere_model > ERB1B_dose_factor).	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.50	3.09. CHEMICAL PROCESSES - TRANSPORT					
2.3.09.51	Atmospheric Transport Through Biosphere	– Radionuclide transport in air, gas, vapor, particulates, aerosols – Processes include: wind, plowing, degassing, precipitation	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.52	Surface Water Transport Through Biosphere	– Radionuclide transport and mixing in surface water – Processes include: lake mixing, river flow, spring discharge, overland flow, irrigation, aeration, sedimentation, dilution [see also Surface Water in 2.3.04.01]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.3.09.53	Soil and Sediment Transport Through Biosphere	– Radionuclide transport in or on soil and sediments – Processes include: fluvial (runoff, river flow), eolian (wind), saltation, glaciation, bioturbation (animals) [see also Erosion in 2.3.07.01, Deposition in 2.3.07.02	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.54	Radionuclide Accumulation in Soils	– Leaching/evaporation from discharge (well, groundwater upwelling) – Deposition from atmosphere or water (irrigation, runoff)	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.55	Recycling of Accumulated Radionuclides from Soils to Groundwater	[see also Radionuclide Release in 2.2.09.65]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.10.00	3.10. BIOLOGICAL PROCESSES					
2.3.10.01	Microbial Activity in Biosphere	– Effect on biosphere characteristics – Effect on transport through biosphere	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.11.00	3.11. THERMAL PROCESSES					
2.3.11.01	Effects of Repository Heat on Biosphere		No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.4.00.00	4. HUMAN BEHAVIOR					
2.4.01.00	4.01. HUMAN CHARACTERISTICS					
2.4.01.01	Human Characteristics	– Physiology – Metabolism – Adults, children [contributes to Radiological Toxicity in 3.3.06.02]	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.4.01.02	Human Evolution	– Changing human characteristics – Sensitization to radiation – Changing lifestyle	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.4.04.00	4.04. LIFESTYLE					
2.4.04.01	Human Lifestyle	– Diet and fluid intake (food, water, tobacco/drugs, etc.) – Dwellings – Household activities – Leisure activities [see also Land and Water Use in 2.4.08.01] [contributes to Ingestion in 3.3.04.01, Inhalation in 3.3.04.02, External Exposure in 3.3.04.03]	Partially	The biosphere model (see model container Results) assumes water intake through a well drilled 5 km down gradient from the repository edge. However, no other aspects of human lifestyle are taken into account. The biosphere model used in the salt GDS model uses a water consumption rate of 1.2 m3/yr for the exposed individual.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.4.08.00	4.08. LAND AND WATER USE					
2.4.08.01	Land and Water Use	– Agricultural (irrigation, plowing, fertilization, crop storage, greenhouses, hydroponics) – Farms and Fisheries (feed, water, soil) – Urban / Industrial (development, energy production, earthworks, population density) – Natural / Wild (grasslands, forests, bush, surface water)	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.4.08.02	Evolution of Land and Water Use	– New practices (agricultural, farming, fisheries) – Technological developments – Social developments (new/expanded communities)	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
3.0.00.00	3. RADIONUCLIDE / CONTAMINANT FACTORS (BIOSPHERE)					
3.1.00.00	1. CONTAMINANT CHARACTERISTICS					
3.2.00.00	2. RELEASE / MIGRATION FACTORS					
3.3.00.00	3. EXPOSURE FACTORS					
3.3.01.00	3.01. RADIONUCLIDE / CONTAMINANT CONCENTRATIONS					
3.3.01.01	Radionuclides in Biosphere Media	– Soil – Surface Water – Air – Plant Uptake – Animal (Livestock, Fish) Uptake – Bioaccumulation [contributions from Radionuclide Release from Geologic Units in 2.2.09.65, Transport Through Biosphere in 2.3.09.51/52/53/54/55]	No	The biosphere analysis (see model container Results) focuses on a single exposure pathway: a drinking water well drilled 5 km down gradient from the edge of the repository. This well penetrates an aquifer that has been contaminated by radionuclides released from the repository. Radionuclides in other exposure pathways are not taken into account.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
3.3.01.02	Radionuclides in Food Products	– Diet and fluid sources (location, degree of contamination, dilution with uncontaminated sources) – Foodstuff and fluid processing and preparation (water filtration, cooking techniques) [see also Land and Water Use in 2.4.08.01, Radionuclides in Biosphere Media in 3.3.01.01]	Partially	The biosphere analysis (see model container Results) focuses on a single exposure pathway: a drinking water well drilled 5 km down gradient from the edge of the repository. This well penetrates an aquifer that has been contaminated by radionuclides released from the repository. Radionuclides in other exposure pathways are not taken into account. The analysis uses dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B). This biosphere analysis is used for all of the GDS models to facilitate comparison of disposal environments. In reality, it is unlikely that groundwater drawn from a bedded salt formation would be potable with significant treatment, and that recharge in the marker beds would sustain withdrawal from the well over a long period of time. The biosphere model used in the salt GDS model uses a dilution rate of 1E4 m3/yr in the aquifer from which a drinking water well withdraws water. The model assumes that the dilution rate in the aquifer is large enough to make the water potable.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
3.3.01.03	Radionuclides in Non-Food Products	– Dwellings (location, building materials and sources, fuel sources) – Household products (clothing and sources, furniture and sources, tobacco, pets) – Biosphere media [see also Land and Water Use in 2.4.08.01, Radionuclides in Biosphere Media in 3.3.01.01]	No	The biosphere analysis (see model container Results) focuses on a single exposure pathway: a drinking water well drilled 5 km down gradient from the edge of the repository. This well penetrates an aquifer that has been contaminated by radionuclides released from the repository. Radionuclides in other exposure pathways are not taken into account.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
3.3.04.00	3.04. EXPOSURE MODES					
3.3.04.01	Ingestion	– Food products – Soil, surface water	Partially	The biosphere analysis (see model container Results) focuses on a single exposure pathway: a drinking water well drilled 5 km down gradient from the edge of the repository. This well penetrates an aquifer that has been contaminated by radionuclides released from the repository. Radionuclides in other exposure pathways are not taken into account.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
3.3.04.02	Inhalation	– Gases and vapors – Suspended particulates (dust, smoke, pollen)	No	The biosphere analysis (see model container Results) focuses on a single exposure pathway: a drinking water well drilled 5 km down gradient from the edge of the repository. This well penetrates an aquifer that has been contaminated by radionuclides released from the repository. Radionuclides in other exposure pathways are not taken into account.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-1. FEPs Mapping of the Salt and Granite GDS Models (continued)

FEP Information			Capability Included in Salt GDS Model		Capability Included in Crystalline (Saturated Granite) GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
3.3.04.03	External Exposure	– Non-Food products – Soil, surface water	No	The biosphere analysis (see model container Results) focuses on a single exposure pathway: a drinking water well drilled 5 km down gradient from the edge of the repository. This well penetrates an aquifer that has been contaminated by radionuclides released from the repository. Radionuclides in other exposure pathways are not taken into account.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
3.3.06.00	3.06. TOXICITY / EFFECTS					
3.3.06.01	Radiation Doses	– Exposure rates (ingestion, inhalation, external exposure) – Dose conversion factors – Gases and vapors – Suspended particulates (dust, smoke, pollen)	Partially	Radiation exposure, or dose, is used as the performance metric of the biosphere analysis (see model container Results). The analysis focuses on a simple system with a single exposure pathway: a drinking water well that is drilled 5 km down gradient from the edge of the repository. This well penetrates an aquifer that has been contaminated by radionuclides released from the repository. The analysis uses dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B). The exposure is based on the consumption rate of the drinking water (Results > ERB1B_Biosphere_model > ERB1_Consumption_rate). Doses from other pathways are not considered.	Partially	The ERB 1B dose conversion factors are used in the Biosphere Model. They are implemented at \Container1\Results\ERB1B_Biosphere_model.
3.3.06.02	Radiological Toxicity and Effects	– Human health effects from radiation doses	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
3.3.06.03	Non-Radiological Toxicity and Effects	– Human health effects from non-radiological toxicity	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
0.0.00.00	0. ASSESSMENT BASIS					
0.1.02.01	Timescales of Concern		Yes	The model user can set the time scale of the assessment. However, the sampled parameters do not change with time.	Yes	Simulations can be run to 1,000,000 yr.
0.1.03.01	Spatial Domain of Concern		Yes	The underlying basis behind the model is a "waste unit cell." Except near the edges, repository designs in general are repeatable configurations of emplaced waste separated by constant distances on the horizontal plane. This symmetry allows for the development of simplified 2D representations of an emplacement location and the surrounding natural media. A wide range of configurations can be modeled using the same overall modeling framework by changing input parameters. The "waste unit cell" is defined by a width, height, and depth. The model assumes 1D radionuclide transport within the EBS and 2D radionuclide transport (x – z plane) in the far field. The domain height (z direction) represents the height to an overlying conductive flow unit (an aquifer) where a swept away boundary condition is applied.	Yes	The zones within the borehole are defined at \Deep_Borehole_Data\Borehole_Data\Borehole_Config.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
0.1.09.01	Regulatory Requirements and Exclusions		No	The clay GDS model does not explicitly consider any regulatory requirements or exclusions. It is designed to be a flexible model capable of considering a variety of scenarios.	No	Some generic elements of the regulatory framework, such as the 1,000,000-yr timescale (FEP 0.1.02.01), are included. However, to the extent that the current framework is specific to Yucca Mountain, it is not applicable to generic modeling of a repository. In addition, there is uncertainty regarding the future framework. Currently, the individual GDS model capabilities are being transitioned into the GPAM. When there is additional clarity in the framework, the GPAM can be analyzed to determine the appropriate changes.
0.1.10.01	Model Issues	– Conceptual model – Mathematical implementation – Geometry and dimensionality – Process coupling – Boundary and initial conditions	Partially	The current version of the model includes the first iteration of work on these issues. As such the issues are mostly addressed at a high level. Future iterations of the model will include more refined implementations.	Partially	The current version of the model includes the first iteration of work on these issues. As such the issues are mostly addressed at a high level. Future iterations of the model will include more refined implementations. The current GDS model does leverage an external deep borehole study with a detailed 3D representation of the system with thermal-hydrologic simulations to generate fluxes for use in the GDS radionuclide transport simulations. Future modeling efforts will address additional model issues.
0.1.10.02	Data Issues	– Parameterization and values – Correlations – Uncertainty	Partially	At this early stage of development, it is important to exercise the model and demonstrate capability. As a result, the forms and values of input parameters simply need to be reasonable representations. In the future when greater rigor is needed, work being done by other parts of the UFD Campaign will be used to inform decisions regarding data issues.	Partially	The current version of the model does include some data analysis. However, future iteration will provide more detailed work on data-related issues.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
1.0.00.00	1. EXTERNAL FACTORS					
1.1.00.00	1. REPOSITORY ISSUES					
1.1.01.01	Open Boreholes	– Site investigation boreholes (open, improperly sealed) – Preclosure and postclosure monitoring boreholes – Enhanced flow pathways from EBS	Partially	The capability to assess a variety of stylized fast path groundwater transport pathways is included in this first iteration of the clay GDS model. For example, scenarios that allow for vertical fast pathways in the far field at different distances between the emplaced waste and the centerline between emplacement locations can be considered, potentially representing hypothetical open boreholes.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.1.02.01	Chemical Effects from Preclosure Operations – In EBS – In EDZ – In Host Rock	– Water contaminants (explosives residue, diesel, organics, etc.) – Water chemistry different than host rock (e.g., oxidizing) – Undesirable materials left – Accidents and unplanned events	No	This FEP is site, design, and operational specific and is not addressed in models for assessing generic media and design concepts. Thus, there are no plans to include this FEP in the GDS models.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.1.02.02	Mechanical Effects from Preclosure Operations – In EBS – In EDZ – In Host Rock	– Creation of excavation-disturbed zone (EDZ) – Stress relief – Boring and blasting effects – Rock reinforcement effects (drillholes) – Accidents and unplanned events – Enhanced flow pathways [see also Evolution of EDZ in 2.2.01.01]	No	This FEP is site, design, and operational specific and is not addressed in models for assessing generic media and design concepts. Thus, there are no plans to include this FEP in the GDS models.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.1.02.03	Thermal-Hydrologic Effects from Preclosure Operations – In EBS – In EDZ – In Host Rock	– Creation of excavation-disturbed zone (EDZ) – Stress relief – Boring and blasting effects – Rock reinforcement effects (drillholes) – Accidents and unplanned events – Enhanced flow pathways [see also Evolution of EDZ in 2.2.01.01]	No	This FEP is site, design, and operational specific and is not addressed in models for assessing generic media and design concepts. Thus, there are no plans to include this FEP in the GDS models.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.1.08.01	Deviations from Design and Inadequate Quality Control	– Error in waste emplacement (waste forms, waste packages, waste package support materials) – Error in EBS component emplacement (backfill, seals, liner) – Inadequate excavation / construction (planning, schedule, implementation) – Aborted / incomplete closure of repository – Material and/or component defects	No	This FEP is design, and operational specific and is not addressed in models for assessing generic media and design concepts. Thus, there are no plans to include this FEP in the GDS models.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.1.10.01	Control of Repository Site	– Active controls (controlled area) – Retention of records – Passive controls (markers)	No	This FEP is policy-specific and is not addressed in models for assessing generic media and design concepts. Thus, there are no plans to explicitly include this FEP in the GDS models.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.1.13.01	Retrievability		No	This FEP is policy-specific and is not addressed in models for assessing generic media and design concepts. Thus, there are no plans to explicitly include this FEP in the GDS models.	No	The disposal system is not amenable to retrievability. It is likely that this FEP is permanently excluded.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.2.00.00	2. GEOLOGICAL PROCESSES AND EFFECTS					
1.2.01.00	2.01. LONG-TERM PROCESSES					
1.2.01.01	Tectonic Activity – Large Scale	– Uplift – Folding	No	This FEP is primarily site specific and pertains to process that occur over very long time periods (geologic time). There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.02	Subsidence		No	This FEP is primarily site specific and pertains to process that occur over very long time periods (geologic time). There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.03	Metamorphism	– Structural changes due to natural heating and/or pressure	No	This FEP is primarily site specific and pertains to process that occur over very long time periods (geologic time). There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.04	Diagenesis	– Mineral alteration due to natural processes	No	This FEP is primarily site specific and pertains to process that occur over very long time periods (geologic time). There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.05	Diapirism	– Plastic flow of rocks under lithostatic loading – Salt/Evaporites – Clay	No	This FEP is primarily site specific and pertains to process that occur over very long time periods (geologic time). There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.01.06	Large-Scale Dissolution		No	This FEP is primarily site specific and pertains to process that occur over very long time periods (geologic time). There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
1.2.03.00	2.03.SEISMIC ACTIVITY					
1.2.03.01	Seismic Activity Impacts EBS and/or EBS Components	– Mechanical damage to EBS (from ground motion, rockfall, drift collapse, fault displacement) [see also Mechanical Impacts in 2.1.07.04, 2.1.07.05, 2.1.07.06, 2.1.07.07, 2.1.07.08, and 2.1.07.10]	Partially	This FEP is site and design specific. There are no plans to explicitly include this FEP. However, this initial version of the clay GDS model allows the user to define EBS barrier properties and performance attributes at a high level, potentially allowing for stylized sensitivity studies to evaluate the effects of seismic activity on EBS components.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.03.02	Seismic Activity Impacts Geosphere – Host Rock – Other Geologic Units	– Altered flow pathways and properties – Altered stress regimes (faults, fractures) [see also Alterations and Impacts in 2.2.05.01, 2.2.05.02, 2.2.05.03, 2.1.07.01, and 2.1.07.02]	Partially	This FEP is site and design specific. There are no plans to explicitly include this FEP. However, this initial version of the clay GDS model allows the user to define far-field properties and performance attributes at a high level, potentially allowing for stylized sensitivity studies to evaluate the effects of seismic activity on far-field components.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.03.03	Seismic Activity Impacts Biosphere – Surface Environment – Human Behavior	– Altered surface characteristic – Altered surface transport pathways – Altered Recharge	No	This FEP is site specific. This initial version of the clay GDS model assumes a stylized biosphere and resultant dose conversion factors based on the IAEA ERB 1B dose model. It does not consider any effects of seismic activity. There are no near-term plans to explicitly consider this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

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Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.2.04.00	2.04. IGNEOUS ACTIVITY					
1.2.04.01	Igneous Activity Impacts EBS and/or EBS Components	– Mechanical damage to EBS (from igneous intrusion) – Chemical interaction with magmatic volatiles – Transport of radionuclides (in magma, pyroclasts, vents) [see also Mechanical Impacts in 2.1.07.04, 2.1.07.05, 2.1.07.06, 2.1.07.07, and 2.1.07.08]	Partially	This FEP is site and design specific. There are no near-term plans to explicitly include this FEP. However, this initial version of the clay GDS model allows the user to define EBS barrier properties and performance attributes at a high level, potentially allowing for stylized sensitivity studies to evaluate the effects of igneous activity on EBS components.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.04.02	Igneous Activity Impacts Geosphere – Host Rock – Other Geologic Units	– Altered flow pathways and properties – Altered stress regimes (faults, fractures) – Igneous intrusions – Altered thermal and chemical conditions [see also Alterations and Impacts in 2.2.05.01, 2.2.05.02, 2.2.05.03, 2.1.07.01, 2.1.07.02, 2.2.09.03, 2.2.11.06 and 2.2.11.07]	Partially	This FEP is site and design specific. There are no plans to explicitly include this FEP. However, this initial version of the clay GDS model allows the user to define far-field properties and performance attributes at a high level, potentially allowing for stylized sensitivity studies to evaluate the effects of igneous activity on far-field components.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.2.04.03	Igneous Activity Impacts Biosphere – Surface Environment – Human Behavior	– Altered surface characteristic – Altered surface transport pathways – Altered recharge – Ashfall and ash redistribution	No	This FEP is site specific. There are no plans to explicitly consider this FEP. This initial version of the clay GDS model assumes a stylized biosphere and resultant dose conversion factors based on the IAEA ERB 1B dose model. It does not consider any effects of seismic activity. There are no near-term plans to explicitly consider this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.3.00.00	3. CLIMATIC PROCESSES AND EFFECTS					
1.3.01.01	Climate Change – Natural – Anthropogenic	– Variations in precipitation and temperature – Long-term global (sea level, …) – Short-term regional and local – Seasonal local (flooding, storms, …) [see also Human Influences on Climate in 1.4.01.01] [contributes to Precipitation in 2.3.08.01, Surface Runoff and Evapotranspiration in 2.3.08.02]	Partially	This FEP is site specific (location). There are no plans to explicitly include this FEP. However, this initial iteration of the clay GDS model allows the user to change advective flow rates in the EBS and far field. This allows for stylized sensitivity studies to assess the potential effect of climate change, with respect to groundwater flow.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.3.04.01	Periglacial Effects	– Permafrost – Seasonal freeze/thaw	No	This FEP is site specific (location). There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.3.05.01	Glacial and Ice Sheet Effects	– Glaciation – Isostatic depression – Melt water	Partially	This FEP is site specific (location). There are no plans to explicitly include this FEP. However, this initial iteration of the clay GDS model allows the user to change advective flow rates in the EBS and far field. This allows for stylized sensitivity studies to assess the potential effect of climate change, with respect to groundwater flow.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.4.00.00	4. FUTURE HUMAN ACTIONS					
1.4.01.01	Human Influences on Climate – Intentional – Accidental	– Variations in precipitation and temperature – Global, regional, and/or local – Greenhouse gases, ozone layer failure [contributes to Climate Change in 1.3.01.01]	Partially	This FEP is beyond the scope of the UFD Campaign and its development of GDS models. There are no plans to explicitly include this FEP. However, this initial iteration of the clay GDS model allows the user to change advective flow rates in the EBS and far field. This allows for stylized sensitivity studies to assess the potential effect of climate change, with respect to groundwater flow.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.4.02.01	Human Intrusion – Deliberate – Inadvertent	– Drilling (resource exploration, …) – Mining / tunneling – Unintrusive site investigation (airborne, surface-based, …) [see also Control of Repository Site in 1.1.10.01]	Partially	This FEP is beyond the scope of the UFD Campaign and its development of GDS models. There are no plans to explicitly include this FEP. The capability to assess a variety of stylized fast path groundwater transport pathways is included in this first iteration of the clay GDS model. This capability could be used to assess the effects of stylized human intrusion scenarios.	No	The current model does not consider the possible consequences of future human intrusion into a deep borehole repository. Existing US regulatory requirements for consideration of human intrusion events are specific to mined repository concepts, and are not applicable to deep boreholes. If the deep borehole concept is selected, it is likely that the regulations would be revised accordingly.
1.4.11.01	Explosions and Crashes from Human Activities	– War – Sabotage – Testing – Resource exploration / exploitation – Aircraft	No	This FEP is beyond the scope of the UFD Campaign and its development of GDS models. There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.5.00.00	5. OTHER					
1.5.01.01	Meteorite Impact	– Cratering, host rock removal – Exhumation of waste – Alteration of flow pathways	No	This FEP is beyond the scope of the UFD Campaign and its development of GDS models. There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
1.5.01.02	Extraterrestrial Events	– Solar systems (supernova) – Celestial activity (sun - solar flares, gamma-ray bursters, moon - earth tides) – Alien life forms	No	This FEP is beyond the scope of the UFD Campaign and its development of GDS models. There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
1.5.03.01	Earth Planetary Changes	– Changes in earth's magnetic field – Changes in earth's gravitational field (tides) – Changes in ocean currents	No	This FEP is beyond the scope of the UFD Campaign and its development of GDS models. There are no plans to explicitly include this FEP.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.0.00.00	2. DISPOSAL SYSTEM FACTORS					
2.1.00.00	1. WASTES AND ENGINEERED FEATURES					
2.1.01.00	1.01. INVENTORY					
2.1.01.01	Waste Inventory – Radionuclides – Nonradionuclides	– Composition – Enrichment / Burn-up	Yes	36 radionuclides are defined in the container :\EBS_and_NearField\EBS_Properties. Half-lives are defined for each radionuclide and several daughters are identified. The model accounts for the in-growth of daughters and isotopic mixing among radionuclides. The radionuclide inventory is defined for each radionuclide through an input spreadsheet, giving flexibility to consider different inventories. The inventory is input into the model at container \Parameters_and_Materials\Input\Waste Form_Input.	Yes	36 radionuclides are defined in the container :\Materials. Half-lives are defined for each radionuclide and several daughters are identified. The model accounts for the in-growth of daughters and isotopic mixing among radionuclides. The container at \RN_Inventory contains the data and calculations related to the three types of waste forms: UNF_Inventory for commercial UNF, DOEHLW_Inventory for existing DHLW, and RWHLW_Inventory for CHLW. The isotopic inventory of the commercial UNF is assumed to be represented by the PWR fuel with a burn-up of 60 GWd/MTIHM and 4.73% enrichment and aged 30 yr after discharge from reactor.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.01.02	Radioactive Decay and Ingrowth	– Decay chains – Decay products – Neutron activation	Yes	Radionuclide decay and in-growth are an inherent part of the GoldSim software capability and used in the clay GDS model. The Species element in container :\EBS_and_NearField\EBS_Properties provides half-lives and decay chains	Yes	The container at :\Materials includes information about 36 species including the half-lives, activities, and daughter products and associated properties. The amounts of different species are contained in *RN_Inventory.*
2.1.01.03	Heterogeneity of Waste Inventory – Waste Package Scale – Repository Scale	– Composition – Enrichment / Burn-up – Damaged Area	Partially	This initial version of the clay GDS model does not explicitly include heterogeneous inventory. The "waste unit cell" conceptual approach considers and "infinite" repository of identical waste packages. Heterogeneity can be evaluated at a high level by executing independent simulations with different inventories and subsequent post-processing of results.	No	The current model assumes only one type of waste per borehole. Thus, heterogeneity of waste inventory is not currently included. However, mixed waste could be included in the future.
2.1.01.04	Interactions Between Co-Located Waste		No	This FEP is design specific and not appropriate for consideration at this stage because specific waste streams, conceptual designs, and loading strategies have not been developed.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.02.00	1.02. WASTE FORM					
2.1.02.01	SNF (Commercial, DOE) Degradation – Alteration / Phase Separation – Dissolution / Leaching – Radionuclide Release	Degradation is dependent on: – Composition – Geometry / Structure – Enrichment / Burn-up – Surface Area – Gap and Grain Fraction – Damaged Area – THC Conditions [see also Mechanical Impact in 2.1.07.06 and Thermal-Mechanical Effects in 2.1.11.06]	Partially	The clay GDS model is flexible and capable of considering a variety of different waste forms. It represents waste form degradation as a fractional degradation rate (yr^{-1}) and assumes congruent release of the contained inventory. The fractional degradation rate is a user input parameter (at container :\Parameters_and_Materials\Input\Waste Form_Input). The model also includes a batch-reactor mixing cell (see container :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Form) with dimensions and properties defined from the user spreadsheet.	Partially	The waste form degradation in the source-term analysis is modeled with the yearly fractional degradation rates (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates in the GDS conditions. All GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. In the current GDS model a constant rate is applied to all waste; no temperature dependence is modeled at this time. (from 2010 GDSE Progress Report) This is implemented in the model at \DBH_RN_release\DBH_WF_release.
2.1.02.02	HLW (Glass, Ceramic, Metal) Degradation – Alteration / Phase Separation – Dissolution / Leaching – Cracking – Radionuclide Release	Degradation is dependent on: – Composition – Geometry / Structure – Surface Area – Damaged / Cracked Area – Mechanical Impact – THC Conditions [see also Mechanical Impact in 2.1.07.07 and Thermal-Mechanical Effects in 2.1.11.06]	Partially	The clay GDS model is flexible and capable of considering a variety of different waste forms. It represents waste form degradation as a fractional degradation rate (yr^{-1}) and assumes congruent release of the contained inventory. The fractional degradation rate is a user input parameter (at container :\Parameters_and_Materials\Input\Waste Form_Input). The model also includes a batch-reactor mixing cell (see container :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Form) with dimensions and properties defined from the user spreadsheet.	Partially	The waste form degradation in the source-term analysis is modeled with the yearly fractional degradation rates (i.e., fraction of remaining waste mass degraded per year), with a distribution that captures potential range of degradation rates in the GDS conditions. All GDS options considered are expected to be in chemically reducing conditions with varying degrees of redox conditions of water in contact with the waste form. In the current GDS model a constant rate is applied to all waste; no temperature dependence is modeled at this time. (from 2010 GDSE Progress Report) This is implemented in the model at \DBH_RN_release\DBH_WF_release.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.02.03	Degradation of Organic/Cellulosic Materials in Waste	[see also Complexation in EBS in 2.1.09.54]	No	It is assumed that organic/cellulosic materials would not be emplaced.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.02.04	HLW (Glass, Ceramic, Metal) Recrystallization		No	See FEP 2.1.02.02. Glass recrystallization is not explicitly modeled.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.02.05	Pyrophoricity or Flammable Gas from SNF or HLW	[see also Gas Explosions in EBS in 2.1.12.04]	No	It is assumed that pyrophoric materials and materials that would generate flammable gas would not be disposed.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.02.06	SNF Cladding Degradation and Failure	– Initial damage – General Corrosion – Microbially Influenced Corrosion – Localized Corrosion – Enhanced Corrosion (silica, fluoride) – Stress Corrosion Cracking – Hydride Cracking – Unzipping – Creep – Internal Pressure – Mechanical Impact	No	The clay GDS model does not consider SNF cladding.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.03.00	1.03. WASTE CONTAINER					
2.1.03.01	Early Failure of Waste Packages	– Manufacturing defects – Improper sealing [see also Deviations from Design in 1.1.08.01]	Partially	The clay GDS model "waste unit cell" approach considers a single primary barrier (waste container). The user can define a time that the primary barrier fails, but does not explicitly consider individual degradation processes and resultant degraded conditions. It is assumed that the primary barrier fails completely at the user-prescribed time. Temporal variability of primary barrier degradation is not considered - the "waste unit cell" approach assumes all an "infinite" repository of identical waste packages and associated performance. The effects of early failure could be evaluated at a high level by changing the time that failure of the primary engineered barrier occurs.	No	It is possible to specify a failure time reflecting early failure. However, the current model assumes waste package failure occurs immediately after emplacement.
2.1.03.02	General Corrosion of Waste Packages	– Dry-air oxidation – Humid-air corrosion – Aqueous phase corrosion – Passive film formation and stability	Partially	The clay GDS model "waste unit cell" approach considers a single primary barrier (waste container). The user can define a time that the primary barrier fails, but does not explicitly consider individual degradation processes and resultant degraded conditions. It is assumed that the primary barrier fails completely at the user-prescribed time. Temporal variability of primary barrier degradation is not considered - the "waste unit cell" approach assumes all an "infinite" repository of identical waste packages and associated performance. General corrosion rates can be used in ancillary calculations to determine the time of primary engineered barrier failure. This time can be changed in the user spreadsheet to evaluate sensitivity.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion. The current model assumes waste package failure occurs immediately after emplacement.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.03.03	Stress Corrosion Cracking (SCC) of Waste Packages	– Crack initiation, growth and propagation – Stress distribution around cracks	Partially	The clay GDS model "waste unit cell" approach considers a single primary barrier (waste container). The user can define a time that the primary barrier fails, but does not explicitly consider individual degradation processes and resultant degraded conditions. It is assumed that the primary barrier fails completely at the user-prescribed time. Temporal variability of primary barrier degradation is not considered - the "waste unit cell" approach assumes all an "infinite" repository of identical waste packages and associated performance. Stress corrosion cracking rates can be used in ancillary calculations to determine the time of primary engineered barrier failure. This time can be changed in the user spreadsheet to evaluate sensitivity. However, such a sensitivity would assume complete failure of the primary engineered barrier, as opposed to limited breaches that would occur due to SCC.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion. The current model assumes waste package failure occurs immediately after emplacement.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.03.04	Localized Corrosion of Waste Packages	– Pitting – Crevice corrosion – Salt deliquescence [see also 2.1.09.06 Chemical Interaction with Backfill]	Partially	The clay GDS model "waste unit cell" approach considers a single primary barrier (waste container). The user can define a time that the primary barrier fails, but does not explicitly consider individual degradation processes and resultant degraded conditions. It is assumed that the primary barrier fails completely at the user-prescribed time. Temporal variability of primary barrier degradation is not considered - the "waste unit cell" approach assumes all an "infinite" repository of identical waste packages and associated performance. Localized corrosion rates can be used in ancillary calculations to determine the time of primary engineered barrier failure. This time can be changed in the user spreadsheet to evaluate sensitivity. However, such a sensitivity would assume complete failure of the primary engineered barrier, as opposed to limited breaches that would occur due to localized corrosion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion. The current model assumes waste package failure occurs immediately after emplacement.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.03.05	Hydride Cracking of Waste Packages	– Hydrogen diffusion through metal matrix – Crack initiation and growth in metal hydride phases	Partially	The clay GDS model "waste unit cell" approach considers a single primary barrier (waste container). The user can define a time that the primary barrier fails, but does not explicitly consider individual degradation processes and resultant degraded conditions. It is assumed that the primary barrier fails completely at the user-prescribed time. Temporal variability of primary barrier degradation is not considered - the "waste unit cell" approach assumes all an "infinite" repository of identical waste packages and associated performance. Hydride cracking rates can be used in ancillary calculations to determine the time of primary engineered barrier failure. This time can be changed in the user spreadsheet to evaluate sensitivity. However, such a sensitivity would assume complete failure of the primary engineered barrier, as opposed to limited breaches that would occur due to hydride cracking.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion. The current model assumes waste package failure occurs immediately after emplacement.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.03.06	Microbially Influenced Corrosion (MIC) of Waste Packages		Partially	The clay GDS model "waste unit cell" approach considers a single primary barrier (waste container). The user can define a time that the primary barrier fails, but does not explicitly consider individual degradation processes and resultant degraded conditions. It is assumed that the primary barrier fails completely at the user-prescribed time. Temporal variability of primary barrier degradation is not considered - the "waste unit cell" approach assumes all an "infinite" repository of identical waste packages and associated performance. MIC enhanced corrosion rates can be used in ancillary calculations to determine the time of primary engineered barrier failure. This time can be changed in the user spreadsheet to evaluate sensitivity.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion. The current model assumes waste package failure occurs immediately after emplacement.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.03.07	Internal Corrosion of Waste Packages Prior to Breach		No	The clay GDS model "waste unit cell" approach considers a single primary barrier (waste container). The user can define a time that the primary barrier fails, but does not explicitly consider individual degradation processes and resultant degraded conditions. It is assumed that the primary barrier fails completely at the user-prescribed time. Temporal variability of primary barrier degradation is not considered - the "waste unit cell" approach assumes all an "infinite" repository of identical waste packages and associated performance. Primary engineered barrier internal corrosion rates can be used in ancillary calculations to determine the time of primary engineered barrier failure. This time can be changed in the user spreadsheet to evaluate sensitivity.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion. The current model assumes waste package failure occurs immediately after emplacement.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.03.08	Evolution of Flow Pathways in Waste Packages	– Evolution of physical form of waste package – Plugging of cracks in waste packages [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Mechanical Impacts in 2.1.07.05, 2.1.07.06, and 2.1.07.07, Thermal-Mechanical Effects in 2.1.11.06 and 2.1.11.07]	Partially	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion. The clay GDS model assumes that when the primary engineered barrier fails, the contained waste form is completely exposed for subsequent degradation. Properties of the degraded waste form and primary engineered barrier are input to the model from the user spreadsheet. These properties are static (do not vary with time), so the time-dependent evolution is not explicitly modeled. However, the user can change these properties to evaluate effects through sensitivity analysis. The degraded waste form component is at container :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Form and the degraded primary engineered barrier component is at container :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Package. Properties are input at containers :\Parameters_and_Materials\Input\WasteForm_Input and :\Parameters_and_Materials\Input\WastePackage_Input.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion. The current model assumes waste package failure occurs immediately after emplacement.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.04.00	1.04. BUFFER / BACKFILL					
2.1.04.01	Evolution and Degradation of Backfill	– Alteration – Thermal expansion / Degradation – Swelling/Compaction – Erosion/Dissolution – Evolution of backfill flow pathways [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Mechanical Impact in 2.1.07.04, Thermal-Mechanical Effects in 2.1.11.08, Chemical Interaction in 2.1.09.06]	Partially	The clay GDS model contains a component model for a secondary engineered barrier that can be used to represent radionuclide transport through either a buffer or backfill. The component model is at container :\EBS_and_NearField\EBS_Transport\Secondary_EBS. The properties are entered through the input spreadsheet (at container :\Parameters_and_Materials\Input\SecondaryEBS_Input). These properties are static (do not vary with time), so the time-dependent evolution is not explicitly modeled. However, the user can change these properties to evaluate effects through sensitivity analysis.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.05.00	1.05. SEALS					
2.1.05.01	Degradation of Seals	– Alteration / Degradation / Cracking – Erosion / Dissolution [see also Mechanical Impact in 2.1.07.08, Thermal-Mechanical Effects in 2.1.11.09, Chemical Interaction in 2.1.09.08]	Partially	The clay GDS model does not explicitly model seals and seal degradation. However, the fast radionuclide transport capabilities consist of a 1D diffusive network between the emplaced waste and an advective far-field pathway. The user can define the properties of both the diffusive and advective components. The fast-path component model is at container :\Fast_Path_Scenario\FastPathSource and the properties are input from the user spreadsheet at container: \Parameters_and_Materials\Input\Fast_Pathway_Input. This construct could be used to evaluate the effects of seal properties at a high level through sensitivity studies.	Partially	Explicit modeling of seal degradation processes has not been included. However, permeabilities can be assigned to the seals to represent various levels of degradation. These permeabilities are included in the GoldSim model implicitly through the calculated flow fields used in the model. There has been a sensitivity analysis considering degradation of seals in terms of increased seal permeability. The high permeability case in the GDS model represents the higher bound case for the sensitivity analysis.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.06.00	1.06. OTHER EBS MATERIALS					
2.1.06.01	Degradation of Liner / Rock Reinforcement Materials in EBS	– Alteration / Degradation / Cracking – Corrosion – Erosion / Dissolution / Spalling [see also Mechanical Impact in 2.1.07.08, Thermal-Mechanical Effects in 2.1.11.09, Chemical Interaction in 2.1.09.07]	No	The conceptual model implemented does not include liner and/or rock reinforcement materials	No	None of these processes are modeled in the Disposal Zone or the Seal Zone.
2.1.07.00	1.07. MECHANICAL PROCESSES					
2.1.07.01	Rockfall	– Dynamic loading (block size and velocity) [see also Mechanical Effects on Host Rock in 2.2.07.01]	No	Rockfall is not expected in a clay disposal environment and it has been assumed not to be important.	No	Rockfall is excluded because the design of the borehole (i.e., backfill) makes it unlikely.
2.1.07.02	– Drift Collapse	– Static loading (rubble volume) – Alteration of seepage – Alteration of EBS flow pathways – Alteration of EBS thermal environment [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Chemical Effects of Drift Collapse in 2.1.09.12, and Effects of Drift Collapse on TH in 2.1.11.04, Mechanical Effects on Host Rock in 2.2.07.01]	No	This FEP is design and site specific - not explicitly considered in the clay GDS model.	No	The deep borehole GDS model does not include any drifts.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.07.03	Mechanical Effects of Backfill	– Protection of other EBS components from rockfall / drift collapse	No	This FEP is design and site specific - not explicitly considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.04	Mechanical Impact on Backfill	– Rockfall / Drift collapse – Hydrostatic pressure – Internal gas pressure [see also Degradation of Backfill in 2.1.04.01 and Thermal-Mechanical Effects in 2.1.11.08]	No	This FEP is design and site specific - not explicitly considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.05	Mechanical Impact on Waste Packages	– Rockfall / Drift collapse – Waste package movement – Hydrostatic pressure – Internal gas pressure – Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.07]	No	This FEP is design and site specific - not explicitly considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.06	Mechanical Impact on SNF Waste Form	– Drift collapse – Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.06]	No	This FEP is design and site specific - not explicitly considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.07	Mechanical Impact on HLW Waste Form	– Drift collapse – Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.06]	No	This FEP is design and site specific - not explicitly considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.07.08	Mechanical Impact on Other EBS Components – Seals – Liner/Rock Reinforcement Materials – Waste Package Support Materials	– Rockfall / Drift collapse – Movement – Hydrostatic pressure – Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.09]	No	This FEP is design and site specific - not explicitly considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.09	Mechanical Effects at EBS Component Interfaces	– Component-to-component contact (static or dynamic)	No	This FEP is design and site specific - not explicitly considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.07.10	Mechanical Degradation of EBS	– Floor buckling – Fault displacement – Initial damage from excavation / construction – Consolidation of EBS components – Degradation of waste package support structure – Alteration of EBS flow pathways [see also Mechanical Effects from Preclosure in 1.1.02.02, Evolution of Flow Pathways in EBS in 2.1.08.06, Drift Collapse in 2.1.07.02, Degradation in 2.1.04.01, 2.1.05.01, and 2.1.06.01, and Mechanical Effects on Host Rock in 2.2.07.01]	No	This FEP is design and site specific - not explicitly considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.08.00	1.08. HYDROLOGIC PROCESSES					
2.1.08.01	Flow Through the EBS	– Saturated / Unsaturated flow – Preferential flow pathways – Density effects on flow – Initial hydrologic conditions – Flow pathways out of EBS [see also Open Boreholes in 1.1.01.01, Thermal-Hydrologic Effects from Preclosure in 1.1.02.03, Flow in Waste Packages in 2.1.08.02, Flow in Backfill in 2.1.08.03, Flow through Seals 2.1.08.04, Flow through Liner in 2.1.08.05, Thermal Effects on Flow in 2.1.11.10, Effects of Gas on Flow in 2.1.12.02]	Yes	The clay GDS model includes 1D advective flow (saturated) linkages between the EBS components: Waste Form → Primary Engineered Barrier → Primary Engineered Barrier → EDZ. These linkages can be found in the batch-reactor mixing cells in the following containers: – Waste Form :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Form – Primary Engineered Barrier :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Package – Secondary Engineered Barrier :\EBS_and_NearField\EBS_Transport\Secondary_EBS The advective flow rate through each barrier is a user input parameter, input from the input spreadsheet. The advective flow rate (m^3/yr) does not vary with time (static value) and is deterministic. Containers where input is defined are: – Waste Form :\Parameters_and_Materials\Input\WasteForm_Input – Primary Engineered Barrier :\Parameters_and_Materials\Input\WastePackage_Input – Secondary Engineered Barrier :\Parameters_and_Materials\Input\SecondaryEBS_Input	Partially	Flow through the Disposal Zone is implemented at \DBH_RN_transport\DBH_Transport_DisposalZone\DisposalZone_MultipleCells. The flow is modeled as fully saturated. Flow through the Seal Zone is implemented in \DBH_RN_transport\DBH_Transport_SealZone\SealZone_MultipleCells. The flow is modeled as fully saturated. The other features and processes identified in this FEP are not modeled.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.08.02	Flow In and Through Waste Packages	– Saturated / Unsaturated flow – Movement as thin films or droplets	Yes	See FEP 2.1.08.01 for discussion (Primary Engineered Barrier)	No	Flow through waste packages is not modeled. The waste packages are modeled as degraded at time zero.
2.1.08.03	Flow in Backfill	– Fracture / Matrix flow	Yes	See FEP 2.1.08.01 for discussion (Secondary Engineered Barrier)	Partially	Flow through the Seal Zone is implemented in \DBH_RN_transport\DBH_Transport_SealZone\SealZone_MultipleCells. Advective and diffusive transport is modeled through the bentonite of the Seal Zone. Fractures are not modeled in the Seal Zone.
2.1.08.04	Flow Through Seals	– Fracture / Matrix flow	Partially	The clay GDS model does not explicitly model seals and flow through seals. However, the fast radionuclide transport capabilities consist of a 1D diffusive network between the emplaced waste and an advective far-field pathway. The user can define the properties of both the diffusive and advective components. The fast-path component model is at container :\Fast_Path_Scenario\FastPathSource and the properties are input from the user spreadsheet at container: \Parameters_and_Materials\Input\Fast_Pathway_Input. This construct could be used to evaluate the effects of flow through seals at a high level through sensitivity studies.	Partially	Flow through the Seal Zone is implemented in \DBH_RN_transport\DBH_Transport_SealZone\SealZone_MultipleCells. Advective and diffusive transport is modeled through the bentonite of the Seal Zone. Fractures are not modeled in the Seal Zone. Gas transport is not implemented.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.08.05	Flow Through Liner / Rock Reinforcement Materials in EBS		No	This clay GDS model does not consider liners/rock reinforcement.	Yes	Flow through the Disposal Zone is implemented at \DBH_RN_transport\DBH_Transport_DisposalZone\DisposalZone_MultipleCells. Advective and diffusive transport is modeled in the Disposal Zone. Flow through the Seal Zone is implemented in \DBH_RN_transport\DBH_Transport_SealZone\SealZone_MultipleCells. Advective and diffusive transport is modeled through the bentonite of the Seal Zone.
2.1.08.06	Alteration and Evolution of EBS Flow Pathways	– Drift collapse – Degradation/consolidation of EBS components – Plugging of flow pathways – Formation of corrosion products – Water ponding [see also Evolution of Flow Pathways in WPs in 2.1.03.08, Evolution of Backfill in 2.1.04.01, Drift Collapse in 2.1.07.02, and Mechanical Degradation of EBS in 2.1.07.10]	Partially	The properties of the EBS components (Waste Form Primary Engineered Barrier, Secondary Engineered Barrier) are user input and no temporal variability is assumed. However, the effects of different EBS flow pathway properties can be assessed at a high level through sensitivity studies.	No	None of these processes are modeled in the Disposal Zone or the Seal Zone.
2.1.08.07	Condensation Forms in Repository – On Tunnel Roof/Walls – On EBS Components	– Heat transfer (spatial and temporal distribution of temperature and relative humidity) – Dripping – Moisture movement [see also Heat Generation in EBS in 2.1.11.01, Effects on EBS Thermal Environment in 2.1.11.03 and 2.1.11.04]	No	The conceptual model of a clay generic environment assumes it is fully saturated and isothermal (ambient temperature).	No	Condensation and evaporation are not relevant to the deep borehole disposal model. Due to extremely high fluid pressures at depths of 3 to 5 km, evaporation is ruled out.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.08.08	Capillary Effects in EBS	– Wicking – Capillary barrier – Osmotic binding	No	The conceptual model of a clay generic environment assumes it is fully saturated and isothermal (ambient temperature).	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.08.09	Influx/Seepage Into the EBS	– Water influx rate (spatial and temporal distribution) [see also Open Boreholes in 1.1.01.01, Thermal Effects on Flow in EBS in 2.1.11.10, Flow Through Host Rock in 2.2.08.01, Effects of Excavation on Flow in 2.2.08.04]	Partially	See FEP 2.1.08.01 for discussion of flow through the EBS (which inherently would assume influx into the EBS.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.00	1.09. CHEMICAL PROCESSES - CHEMISTRY					
2.1.09.01	Chemistry of Water Flowing into the Repository	– Chemistry of influent water (spatial and temporal distribution) [See also Chemistry in Host Rock 2.2.09.01]	No	Far-field groundwater chemistry is not included.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.02	Chemical Characteristics of Water in Waste Packages	– Water composition (radionuclides, dissolved species, …) – Initial void chemistry (air / gas) – Water chemistry (pH, ionic strength, pCO2, …) – Reduction-oxidation potential – Reaction kinetics – Influent chemistry (from tunnels and/or backfill) [see also Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04] – Evolution of water chemistry / interaction with waste packages	Partially	The chemical characteristics of water in the waste packages are not explicitly represented. However, the user does have the ability to input that describes probability distributions for dissolved concentration limits and distribution coefficients in each engineered barrier. As such, the effects of differing chemical characteristics in the waste packages could be assessed through high-level sensitivity studies.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.03	Chemical Characteristics of Water in Backfill	– Water composition (radionuclides, dissolved species, …) – Water chemistry (pH, ionic strength, pCO2, …) – Reduction-oxidation potential – Reaction kinetics – Influent chemistry (from tunnels and/or waste packages) [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Tunnels in 2.1.09.04] – Evolution of water chemistry / interaction with backfill	Partially	The chemical characteristics of water in the backfill (or buffer) are not explicitly represented. However, the user does have the ability to input that describes probability distributions for dissolved concentration limits and distribution coefficients in each engineered barrier. As such, the effects of differing chemical characteristics in a backfill/buffer could be assessed through high-level sensitivity studies.	Partially	The model does not explicitly consider the chemical characteristics of water in the backfill. However, it is partially included through the effects of water chemistry on solubility and sorption. Solubility limits for the Seal Zone are defined at \Uncertain_Parameters\RN_Solubility and they are implemented at \DBH_RN_transport\DBH_Transport_SealZone. Some radionuclides are modeled with unlimited solubility. Sorption coefficients for the Seal Zone are defined at \Uncertain_Parameters\DBH_transport_Parameters\DBH_Kd_data\DBH_Kd_SealZone and they are implemented at \DBH_RN_transport\DBH_Transport_SealZone. Some radionuclides are modeled with sorption coefficients set equal to zero.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.04	Chemical Characteristics of Water in Tunnels	– Water composition (radionuclides, dissolved species, …) – Water chemistry (pH, ionic strength, pCO2, …) – Reduction-oxidation potential – Reaction kinetics – Influent chemistry (from construction / emplacement) – Initial chemistry (from construction/emplacement) [see also Chemical Effects from Preclosure in 1.1.02.01, Chemistry of Water Flowing in 2.1.09.01, Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03] – Evolution of water chemistry / interaction with seals, liner/rock reinforcement materials, waste package support materials	Partially	The chemical characteristics of water in the emplacement tunnel (or borehole, room) are not explicitly represented. However, the user does have the ability to input that describes probability distributions for dissolved concentration limits and distribution coefficients in each engineered barrier. As such, the effects of differing chemical characteristics in tunnels could be assessed through high-level sensitivity studies.	No	There are no tunnels in the deep borehole GDS model.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.05	Chemical Interaction of Water with Corrosion Products – In Waste Packages – In Backfill – In Tunnels	– Corrosion product formation and composition (waste form, waste package internals, waste package) – Evolution of water chemistry in waste packages, in backfill, and in tunnels [contributes to Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	This FEP is site and design specific. It is not considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.06	Chemical Interaction of Water with Backfill – On Waste Packages – In Backfill – In Tunnels	– Backfill composition and evolution (bentonite, crushed rock, ...) – Evolution of water chemistry in backfill and in tunnels – Enhanced degradation of waste packages (crevice corrosion) [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04, Localized Corrosion of WPs in 2.1.03.04]	No	This FEP is site and design specific. It is not considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.07	Chemical Interaction of Water with Liner / Rock Reinforcement and Cementitious Materials in EBS – In Backfill – In Tunnels	– Liner composition and evolution (concrete, metal, ...) – Rock reinforcement material composition and evolution (grout, rock bolts, mesh, ….) – Other cementitious materials composition and evolution – Evolution of water chemistry in backfill, and in tunnels [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	This FEP is site and design specific. It is not considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.08	Chemical Interaction of Water with Other EBS Components – In Waste Packages – In Tunnels	– Seals composition and evolution – Waste Package Support composition and evolution (concrete, metal, …) – Other EBS components (other metals - Copper, …) – Evolution of water chemistry in backfill and in tunnels [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	This FEP is site and design specific. It is not considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.09	Chemical Effects at EBS Component Interfaces	– Component-to-component contact (chemical reactions) – Consolidation of EBS components	No	This FEP is site and design specific. It is not considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.10	Chemical Effects of Waste-Rock Contact	– Waste-to-host rock contact (chemical reactions) – Component-to-host rock contact (chemical reactions)	No	This FEP is site and design specific. It is not considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.11	Electrochemical Effects in EBS	– Enhanced metal corrosion	No	This FEP is site and design specific. It is not considered in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.12	Chemical Effects of Drift Collapse	– Evolution of water chemistry in backfill and in tunnels (from altered seepage, from altered thermal-hydrology) [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	Drift collapse is not anticipated in a clay disposal environment.	No	Drift collapse is excluded because the design of the borehole (i.e., backfill) makes it unlikely. Therefore, chemical effects of drift collapse are also excluded.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.13	Radionuclide Speciation and Solubility in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Dissolved concentration limits – Limited dissolution due to inclusion in secondary phase – Enhanced dissolution due to alpha recoil [controlled by Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	Partially	Dissolved concentration limits are represented as log-triangular distributions with the parameters that define the distribution being user inputs. Dissolved concentration limits can be defined independently for each engineered barrier (Waste Form, Primary Engineered Barrier, Secondary Engineered Barrier, and EDZ). The sampled dissolved concentration limits are assumed not to vary with time and do not depend on the EBS environment (which is not explicitly modeled). Containers where the distribution parameters are input to the model are: – Waste Form :\Parameters_and_Materials\Input\WasteForm_Input – Primary Engineered Barrier :\Parameters_and_Materials\Input\WastePackage_Input – Secondary Engineered Barrier :\Parameters_and_Materials\Input\SecondaryEBS_Input The sampled values are determined in container :\Parameters_and_Materials\Epistemic_Parameters	Partially	Solubility limits for the Disposal Zone are defined at \Uncertain_Parameters\RN_Solubility and they are implemented at \DBH_RN_transport\DBH_Transport_DisposalZone. Some radionuclides are modeled with unlimited solubility. It is too early in the development of the model to have the other features and processes implemented in the model. There is no tunnel in the deep borehole GDS model.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.09.50	1.09. CHEMICAL PROCESSES - TRANSPORT					
2.1.09.51	Advection of Dissolved Radionuclides in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Flow pathways and velocity – Advective properties (porosity, tortuosity) – Dispersion – Saturation [see also Gas Phase Transport in 2.1.12.03]	Yes	The clay GDS model includes 1D advective transport (saturated) linkages between the EBS components (batch reactor mixing cells): Waste Form → Primary Engineered Barrier → Primary Engineered Barrier → EDZ. The advective connections can be found in the batch-reactor mixing cells in the following containers: – Waste Form :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Form – Primary Engineered Barrier :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Package – Secondary Engineered Barrier :\EBS_and_NearField\EBS_Transport\Secondary_EBS The advective flow rate through each barrier is a user input parameter, input from the input spreadsheet. The advective flow rate (m^3/yr) does not vary with time (static value) and is deterministic. Containers where input is defined are: – Waste Form :\Parameters_and_Materials\Input\WasteForm_Input – Primary Engineered Barrier :\Parameters_and_Materials\Input\WastePackage_Input – Secondary Engineered Barrier :\Parameters_and_Materials\Input\SecondaryEBS_Input	Yes	Advective transport of dissolved radionuclides is implemented at \DBH_RN_transport\DBH_Transport_DisposalZone\DisposalZone_MultipleCells\DisposalZone_Transport. The Disposal Zone of the Deep Borehole is being mapped to EBS FEPs. The Disposal Zone is filled with filling material defined by the Medium_Disposal_Zone solid element. The waste form is modeled using a fractional degradation rate that provides a source term for advective transport through the filling material defined by the Medium_Disposal_Zone solid element. There is no tunnel in the deep borehole GDS model. Waste packages provide no performance in the deep borehole GDS model.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.52	Diffusion of Dissolved Radionuclides in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Gradients (concentration, chemical potential) – Diffusive properties (diffusion coefficients) – Flow pathways and velocity – Saturation	Yes	The clay GDS model includes 1D diffusive transport (saturated) linkages between the EBS components (batch reactor mixing cells): Waste Form $\rightarrow$ Primary Engineered Barrier $\rightarrow$ Primary Engineered Barrier $\rightarrow$ EDZ. The diffusive connections can be found in the batch-reactor mixing cells in the following containers: – Waste Form :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Form – Primary Engineered Barrier :\EBS_and_NearField\EBS_Transport\Degraded_Waste_Package – Secondary Engineered Barrier :\EBS_and_NearField\EBS_Transport\Secondary_EBS The Secondary Engineered Barrier model includes the capability to represent either single- or dual-continuum radionuclide transport with the dual-continuum model including matrix diffusion. The diffusive properties of each barrier (diffusive length, diffusive area, porosity, tortuosity - secondary engineered barrier, and available porosity - secondary engineered barrier) are user input parameters, input from the input spreadsheet. These properties do not vary with time (static value) and are a combination of deterministic and stochastic parameters. Containers where input is defined are: – Waste Form :\Parameters_and_Materials\Input\WasteForm_Input	Yes	Diffusive transport of dissolved radionuclides is implemented at \DBH_RN_transport\DBH_Transport_DisposalZone\DisposalZone_MultipleCells\DisposalZone_Transport. The Disposal Zone of the Deep Borehole is being mapped to EBS FEPs. The Disposal Zone is filled with filling material defined by the Medium_Disposal_Zone solid element. The waste form is modeled using a fractional degradation rate that provides a source term for diffusive transport through the filling material defined by the Medium_Disposal_Zone solid element. There is no tunnel in the deep borehole GDS model. Waste packages provide no performance in the deep borehole GDS model.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
				– Primary Engineered Barrier :\Parameters_and_Materials\Input\WastePackage_Input – Secondary Engineered Barrier :\Parameters_and_Materials\Input\SecondaryEBS_Input Stochastic parameters are sampled in container :\Parameters_and_Materials\Epistemic_Parameters The effective diffusion coefficient is determined from the free diffusion coefficient of water and the relative diffusivity of each element in water, which are user input values from the input spreadsheet. These are input to the model in container :\Parameters_and_Materials\Input\Free_Diffusion		

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			**Capability Included in Clay/Shale GDS Model**		**Capability Included in Deep Borehole GDS Model**	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.53	Sorption of Dissolved Radionuclides in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Surface complexation properties – Flow pathways and velocity – Saturation [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	Yes	Distribution coefficients (reversible sorption) are represented as log-triangular distributions with the parameters that define the distribution being user inputs. Distribution coefficients can be defined independently for each engineered barrier (Waste Form, Primary Engineered Barrier, Secondary Engineered Barrier, and EDZ). The sampled distribution coefficients are assumed not to vary with time and do not depend on the EBS environment (which is not explicitly modeled). Containers where the distribution parameters are input to the model are: – Waste Form :\Parameters_and_Materials\Input\WasteForm_Input – Primary Engineered Barrier :\Parameters_and_Materials\Input\WastePackage_Input – Secondary Engineered Barrier :\Parameters_and_Materials\Input\SecondaryEBS_Input The sampled values are determined in container :\Parameters_and_Materials\Epistemic_Parameters	Partially	The sorption coefficients for the Disposal Zone are defined at \Uncertain_Parameters\DBH_transport_Parameters\DBH_Kd_data\DBH_Kd_Disposalzone. Some radionuclides are modeled with sorption coefficients set equal to zero.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.54	Complexation in EBS	– Formation of organic complexants (humates, fulvates, organic waste) – Enhanced transport of radionuclides associated with organic complexants [see also Degradation of Organics in Waste in 2.1.02.03; see Radionuclide Speciation in 2.1.09.13 for inorganic complexation]	No	It was assumed that no organic complexation would occur in the EBS.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.55	Formation of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Formation of intrinsic colloids – Formation of pseudo colloids (host rock fragments, waste form fragments, corrosion products, microbes) – Formation of co-precipitated colloids – Sorption/attachment of radionuclides to colloids (clay, silica, waste form, FeOx, microbes)	No	Colloidal radionuclide transport was not considered in this version of the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.56	Stability of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Chemical stability of attachment (dependent on water chemistry) – Mechanical stability of colloid (dependent on colloid size, gravitational setting)	No	Colloidal radionuclide transport was not considered in this version of the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.57	Advection of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Flow pathways and velocity – Advective properties (porosity, tortuosity) – Dispersion – Saturation – Colloid concentration	No	Colloidal radionuclide transport was not considered in this version of the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.58	Diffusion of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Gradients (concentration, chemical potential) – Diffusive properties (diffusion coefficients) – Flow pathways and velocity – Saturation – Colloid concentration	No	Colloidal radionuclide transport was not considered in this version of the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.59	Sorption of Colloids in EBS – In Waste Form – In Waste Package – In Backfill – In Tunnel	– Surface complexation properties – Flow pathways and velocity – Saturation – Colloid concentration [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	No	Colloidal radionuclide transport was not considered in this version of the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.60	Sorption of Colloids at Air-Water Interface in EBS		No	Colloidal radionuclide transport was not considered in this version of the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.09.61	Filtration of Colloids in EBS	– Physical filtration or trapping (dependent on flow pathways, colloid size) – Electrostatic filtration	No	Colloidal radionuclide transport was not considered in this version of the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.62	Radionuclide Transport Through Liners and Seals	– Advection – Dispersion – Diffusion – Sorption [contributes to Radionuclide release from EBS in 2.1.09.63]	Partially	The clay GDS model does not explicitly model seals and radionuclide transport through seals. However, the fast radionuclide transport capabilities consist of a 1D diffusive network between the emplaced waste and an advective far-field pathway. The user can define the properties of both the diffusive and advective components. The fast-path component model is at container :\Fast_Path_Scenario\FastPathSource and the properties are input from the user spreadsheet at container: \Parameters_and_Materials\Input\Fast_Pathway_Input. This construct could be used to evaluate the effects of flow through seals at a high level through sensitivity studies.	Yes	Advective and diffusive transport of dissolved radionuclides is implemented at \DBH_RN_transport\DBH_Transport_SealZone. The Seal Zone of the DBH Model is being mapped to this FEP. Sorption coefficients for the Seal Zone are defined at \Uncertain_Parameters\DBH_transport_Parameters\DBH_Kd_data\DBH_Kd_SealZone and they are implemented at \DBH_RN_transport\DBH_Transport_SealZone. Some radionuclides are modeled with sorption coefficients set equal to zero. In addition, for a sensitivity analysis Iodine is modeled with sorption due to gettering.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.09.63	Radionuclide Release from the EBS – Dissolved – Colloidal – Gas Phase	– Spatial and temporal distribution of releases to the host rock (due to varying flow pathways and velocities, varying component degradation rates, varying transport properties) [contributions from Dissolved in 2.1.09.51/52/53, Colloidal in 2.1.09.57/58/59, Gas Phase in 2.1.12.03, Liners and Seals in 2.1.09.62]	Partially	See FEPs 2.1.09.51 and 2.1.09.52. Radionuclides released from the EBS enter the EDZ component of the clay GDS model (dissolved species only).	Partially	The radionuclide releases from the Disposal Zone are collected at \DBH_RN_transport\DBH_Transport_DisposalZone\DisposalZone_MultipleCells\DisposalZone_Transport\DisposalZone_5000_4000\DZCell_4200_4000. The mass flux of individual radionuclides at the top of the Disposal Zone is calculated. The radionuclide releases at the top of the Seal Zone are collected at \DBH_RN_transport\DBH_Transport_SealZone\SealZone_MultipleCells\SealZone_Transport\SealZone_3000_2000\SZCell_2100_2000. The mass flux of individual radionuclides at the top of the Seal Zone is calculated. Colloids are not included in the deep borehole GDS model. Gas phase transport is not included in the deep borehole GDS model, because evaporation is not likely.
2.1.10.00	1.10. BIOLOGICAL PROCESSES					
2.1.10.01	Microbial Activity in EBS – Natural – Anthropogenic	– Effects on corrosion – Formation of complexants – Formation of microbial colloids – Formation of biofilms – Biodegradation – Biomass production – Bioaccumulation [see also Microbially Influenced Corrosion in 2.1.03.06, Complexation in EBS in 2.1.09.54, Radiological Mutation of Microbes in 2.1.13.03]	No	Microbial activity in the EBS is not considered.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.11.00	1.11. THERMAL PROCESSES					
2.1.11.01	Heat Generation in EBS	– Heat transfer (spatial and temporal distribution of temperature and relative humidity) [see also Thermal-Hydrologic Effects from Preclosure in 1.1.02.03, Waste Inventory in 2.1.01.01]	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	Partially	The Disposal Zone is assumed to be at 100°C in the deep borehole GDS model. This temperature is used to determine solubility coefficients in the Disposal Zone. Heat generation and associated thermal-hydrologic effects the disposal zone are explicitly modeled in a 3D process model. However, only the resulting vertical ground water fluxes through the borehole are used in the GDS model. Future modeling will include temperature effects on other inputs to the GDS model.
2.1.11.02	Exothermic Reactions in EBS	– Oxidation of SNF – Hydration of concrete	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.11.03	Effects of Backfill on EBS Thermal Environment	– Thermal blanket – Condensation	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	No	There are no near-term plans to include this FEP. Condensation is not relevant to the deep borehole disposal model as pressures at such a depth are much higher than saturation.
2.1.11.04	Effects of Drift Collapse on EBS Thermal Environment	– Thermal blanket – Condensation	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	No	Drift collapse is excluded because the design of the borehole (i.e., backfill) makes it unlikely. Condensation is not relevant to the deep borehole disposal model as pressures at such a depth are much higher than saturation. Therefore, the effects of drift collapse on the EBS thermal environment are also excluded.
2.1.11.05	Effects of Influx (Seepage) on Thermal Environment	– Temperature and relative humidity (spatial and temporal distribution) [see also Influx/Seepage into EBS in 2.1.08.09]	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.11.06	Thermal-Mechanical Effects on Waste Form and In-Package EBS Components	– Alteration – Cracking – Thermal expansion / stress	Partially	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. The waste form properties are user inputs that could be changed to evaluate potential impacts of thermal-mechanical induced property changes through high-level sensitivity studies.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.11.07	Thermal-Mechanical Effects on Waste Packages	– Thermal sensitization / phase changes – Cracking – Thermal expansion / stress/ creep	Partially	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. The primary engineered barrier properties are user inputs that could be changed to evaluate potential impacts of thermal-mechanical induced property changes through high-level sensitivity studies.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.11.08	Thermal-Mechanical Effects on Backfill	– Alteration – Cracking – Thermal expansion / stress	Partially	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. The secondary engineered barrier properties are user inputs that could be changed to evaluate potential impacts of thermal-mechanical induced property changes through high-level sensitivity studies.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.11.09	Thermal-Mechanical Effects on Other EBS Components – Seals – Liner / Rock Reinforcement Materials – Waste Package Support Structure	– Alteration – Cracking – Thermal expansion / stress	Partially	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. The clay GDS model does not explicitly model seals and seal degradation. However, the fast radionuclide transport capabilities consist of a 1D diffusive network between the emplaced waste and an advective far-field pathway. The user can define the properties of both the diffusive and advective components. The fast-path component model is at container :\Fast_Path_Scenario\FastPathSource and the properties are input from the user spreadsheet at container: \Parameters_and_Materials\Input\Fast_Pathway_Input. This construct could be used to evaluate the thermal-mechanical effects of seal properties at a high level through sensitivity studies.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.11.10	Thermal Effects on Flow in EBS	– Altered influx/seepage – Altered saturation / relative humidity (dry-out, resaturation) – Condensation	Partially	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. Flow through the EBS is discussed in FEP 2.1.08.01. The thermal effects on flow could be assessed through high-level sensitivity studies by varying the advective flow rates through the EBS.	Partially	The Disposal Zone is assumed to be at 100°C in the deep borehole GDS model. This temperature is used to determine solubility coefficients in the Disposal Zone. Heat generation and associated thermal-hydrologic effects in the disposal zone are explicitly modeled in a 3D process model. However, only the resulting vertical ground water fluxes through the borehole are used in the deep borehole GDS model. Future modeling will include temperature and other inputs to the deep borehole GDS model.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.1.11.11	Thermally-Driven Flow (Convection) in EBS	– Convection	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. The environment is assumed to be fully saturated.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.11.12	Thermally-Driven Buoyant Flow / Heat Pipes in EBS	– Vapor flow	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. The environment is assumed to be fully saturated.	Partially	Heat generation and associated thermal-hydrologic effects in the disposal zone are explicitly modeled in a 3D process model. However, only the resulting vertical ground water fluxes through the borehole are used in the GDS model. However, heat pipes are not included. There is no vapor formation in the deep borehole system because of the high fluid pressures at depth.
2.1.11.13	Thermal Effects on Chemistry and Microbial Activity in EBS		No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. The environment is assumed to be fully saturated.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.11.14	Thermal Effects on Transport in EBS	– Thermal diffusion (Soret effect) – Thermal osmosis	Partially	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed. Flow through the EBS is discussed in FEP 2.1.08.01. Radionuclide transport through the EBS is discussed in FEPs 2.1.09.51 and 2.1.09.52. The thermal effects on radionuclide transport could be assessed through high-level sensitivity studies by varying the advective flow rates through the EBS and EBS diffusive properties.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.12.00	1.12. GAS SOURCES AND EFFECTS					
2.1.12.01	Gas Generation in EBS	– Repository Pressurization – Mechanical Damage to EBS Components – He generation from waste from alpha decay – H_2 generation from waste package corrosion – CO_2, CH_4, and H_2S generation from microbial degradation – Vaporization of water	No	Gas generation and its effect on the EBS are not included in the model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.12.02	Effects of Gas on Flow Through the EBS	– Two-phase flow – Gas bubbles [see also Buoyant Flow/Heat Pipes in 2.1.11.12]	No	Gas generation and its effect on the EBS are not included in the model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.12.03	Gas Transport in EBS	– Gas phase transport – Gas phase release from EBS	No	Gas generation and its effect on the EBS are not included in the model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.12.04	Gas Explosions in EBS	[see also Flammable Gas from Waste in 2.1.02.05]	No	Gas generation and its effect on the EBS are not included in the model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.13.00	1.13. RADIATION EFFECTS					
2.1.13.01	Radiolysis – In Waste Package – In Backfill – In Tunnel	– Gas generation – Altered water chemistry	No	Radiolysis is not considered in the model	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.1.13.02	Radiation Damage to EBS Components – Waste Form – Waste Package – Backfill – Other EBS Components	– Enhanced waste form degradation – Enhanced waste package degradation – Enhanced backfill degradation – Enhanced degradation of other EBS components (liner/rock reinforcement materials, seals, waste support structure)	No	Radiation damage to EBS components is not considered in the model	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.13.03	Radiological Mutation of Microbes		No	Radiological mutation of microbes and the associated effects on EBS components is not considered in the model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.14.00	1.14. NUCLEAR CRITICALITY					
2.1.14.01	Criticality In-Package	– Formation of critical configuration	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.1.14.02	Criticality in EBS or Near-Field	– Formation of critical configuration	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.00.00	2. GEOLOGICAL ENVIRONMENT					
2.2.01.00	2.01. EXCAVATION DISTURBED ZONE (EDZ)					
2.2.01.01	Evolution of EDZ	– Lateral extent, heterogeneities – Physical properties – Flow pathways – Chemical characteristics of groundwater in EDZ – Radionuclide speciation and solubility in EDZ – Thermal-mechanical effects – Thermal-chemical alteration [see also Mechanical Effects of Excavation in 1.1.02.02]	Yes	The clay GDS model contains a component model for the EDZ that can be used to represent radionuclide transport through it. The component model is at container :\EBS_and_NearField\EBS_Transport\Excavation_Damage_Zone. The properties are entered through the input spreadsheet (at container :\Parameters_and_Materials\Input\EDZ_Input). These properties are static (do not vary with time), so the time-dependent evolution is not explicitly modeled. However, the user can change these properties to evaluate effects through sensitivity analysis. The EDZ model includes the capability to represent either single- or dual-continuum radionuclide transport with the dual-continuum model including matrix diffusion. The user can enter an advective volumetric flow rate through the EDZ. The diffusive properties of the EDZ (diffusive length, diffusive area, porosity, tortuosity - secondary engineered barrier, and available porosity) are user input parameters, input from the input spreadsheet. These properties do not vary with time (static value) and are a combination of deterministic and stochastic parameters. The effective diffusion coefficient is determined from the free diffusion	Partially	Disturbed rock zone (EDZ) does exist in the deep borehole. However, it is not explicitly modeled. It is coupled with the seal zone. Flow through the Seal Zone is implemented in \DBH_RN_transport\DBH_Transport_SealZone\SealZone_MultipleCells. Advective and diffusive transport is modeled through the bentonite of the Seal Zone. Solubility limits for the Seal Zone are defined at \Uncertain_Parameters\RN_Solubility and they are implemented at \DBH_RN_transport\DBH_Transport_SealZone. Some radionuclides are modeled with unlimited solubility. It is too early in the development of the model to have the other features and processes implemented in the model.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
				coefficient of water and the relative diffusivity of each element in water, which are user input values from the input spreadsheet. These are input to the model in container :\Parameters_and_Materials\Input\Free_Diffusion Dissolved concentration limits are represented as log-triangular distributions with the parameters that define the distribution being user inputs. The sampled dissolved concentration limits are assumed not to vary with time and do not depend on the EDZ environment (which is not explicitly modeled). Distribution coefficients (reversible sorption) are represented as log-triangular distributions with the parameters that define the distribution being user inputs. The sampled distribution coefficients are assumed not to vary with time and do not depend on the EDZ environment (which is not explicitly modeled). Containers where input is defined is :\Parameters_and_Materials\Input\EDZ_Input Stochastic parameters are sampled in container :\Parameters_and_Materials\Epistemic_Parameters		

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.02.00	2.02. HOST ROCK					
2.2.02.01	Stratigraphy and Properties of Host Rock	– Rock units – Thickness, lateral extent, heterogeneities, discontinuities, contacts – Physical properties – Flow pathways [see also Fractures in 2.2.05.01 and Faults in 2.2.05.02]	Yes	The far-field component of the clay GDS model i consists of 20x20 node network of batch-reactor mixing cells used to represent 2D radionuclide transport. Releases from the near field enter the far field at the corner of the far-field cell network. Radionuclide transport is assumed to occur primarily via diffusive mechanisms. However, the model includes advective coupling between the mixing cells to evaluate sensitivity. The far-field domain height, width, and depth are represented parametrically within the model and are defined by the user. The model is extremely flexible and can accommodate different repository configurations (e.g., spacing of emplaced waste). Thermal modeling and analysis tools could be used to determine allowable configurations for a prescribed waste form and conceptual repository design that would then be input into the model. The porosity, density, and tortuosity of the far-field media are represented as triangular distributions with the minimum, most likely, and maximum values being user-defined input parameters. Different values for tortuosity can be defined in the horizontal and vertical directions to represent anisotropic diffusive radionuclide transport. The far-field component model is in container :\Far_Field. Input is entered into the model at container :\Parameters_and_Materials\Input\Far_Fi	Partially	The 3D process model that is used to calculate flow rates in the borehole does include the host rock and the combined seal + EDZ as stratigraphic rock units. However, the GDS model does not explicitly include the host rock and other stratigraphic units.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
				eld_Input. Epistemic parameters are sampled at container :\Parameters_and_Materials\Epistemic_Parameters		
2.2.03.00	2.03. OTHER GEOLOGIC UNITS					
2.2.03.01	Stratigraphy and Properties of Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	– Rock units – Thickness, lateral extent, heterogeneities, discontinuities, contacts – Physical properties – Flow pathways [see also Fractures in 2.2.05.01 and Faults in 2.2.05.02]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	Partially	The model includes representations for three segments of a Deep Borehole, a Disposal Zone, a Seal Zone, and an Upper Zone. The model does not include any stratigraphic rock units. For the purposes of FEP analysis the Upper Zone of the Borehole is being equated with the far-field Aquifer. Physical properties of the Upper Zone are defined at \Deep_Borehole_Data\Borehole_Data\DBH_PropertyData.
2.2.05.00	2.05. FLOW AND TRANSPORT PATHWAYS					
2.2.05.01	Fractures – Host Rock – Other Geologic Units	– Rock properties [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01]	No	Clay formations considered for geologic disposal are not fractured. This is assumed in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.05.02	Fractures – Host Rock – Other Geologic Units	– Rock properties [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01]	No	Clay formations considered for geologic disposal are not fractured. This is assumed in the clay GDS model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.05.03	Alteration and Evolution of Geosphere Flow Pathways – Host Rock – Other Geologic Units	– Changes In rock properties – Changes in faults – Changes in fractures – Plugging of flow pathways – Changes in saturation [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01, Fractures in 2.2.05.01, and Faults in 2.2.05.02] [see also Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07]	Partially	The clay GDS model allows the user to define a vertical advective flow rate that does not vary with time. The clay GDS model also includes the ability to include vertical advective transport within the far field at 25%, 50%, 75%, and 100% of the domain width within the 20x20 node network. This allows for the simulation of fast paths that do not directly intersect the emplaced waste or the engineered barriers, but could degrade the isolation capability of the far field. The user is able to define the Darcy velocity in these fast paths along with a time and duration that the increased flow occurs.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.07.00	2.07. MECHANICAL PROCESSES					
2.2.07.01	Mechanical Effects on Host Rock	– From subsidence – From salt creep – From clay deformation – From granite deformation (rockfall / drift collapse into tunnels – Chemical precipitation/ dissolution – Stress regimes [see also Subsidence in 1.2.02.01, Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07]	No	It is assumed that there are no mechanical effects on the host rock.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.07.02	Mechanical Effects on Other Geologic Units	– From subsidence – Chemical precipitation / dissolution – Stress regimes [see also Subsidence in 1.2.02.01, Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.08.00	2.08. HYDROLOGIC PROCESSES					
2.2.08.01	Flow Through the Host Rock	– Saturated flow – Fracture flow / matrix imbibition – Unsaturated flow (fingering, capillarity, episodicity, perched water) – Preferential flow pathways – Density effects on flow – Flow pathways in Host Rock [see also Influx/Seepage into EBS in 2.1.08.09, Alteration of Flow Pathways in 2.2.05.03, Thermal Effects on Flow in 2.2.11.01, Effects of Gas on Flow in 2.2.12.02]	No	The clay GDS model allows the user to define a vertical advective flow rate that does not vary with time. The clay GDS model also includes the ability to include vertical advective transport within the far field at 25%, 50%, 75%, and 100% of the domain width within the 20x20 node network. This allows for the simulation of fast paths that do not directly intersect the emplaced waste or the engineered barriers, but could degrade the isolation capability of the far field. The user is able to define the Darcy velocity in these fast paths along with a time and duration that the increased flow occurs.	partially	The 3D process model that is used to calculate flow rates in the borehole does include the host rock and the combined seal + EDZ as stratigraphic rock units. The other features are not implemented.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.08.02	Flow Through the Other Geologic Units – Confining units – Aquifers	– 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 [see also Alteration of Flow Pathways in 2.2.05.03, Thermal Effects on Flow in 2.2.11.01, Effects of Gas on Flow in 2.2.12.02]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	Partially	Flow through the Upper Zone of the Borehole is implemented at \DBH_RN_transport\DBH_Transport_UpperZone\UpperBHZone_Pipe. Saturated flow is modeled. Fracture flow, matrix imbibition and unsaturated flow are not implemented.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.08.03	Effects of Recharge on Geosphere Flow – Host Rock – Other Geologic Units	– Infiltration rate – Water table rise/decline [see also Infiltration 2.3.08.03]	Partially	Recharge is not explicitly modeled. The clay GDS model allows the user to define a vertical advective flow rate that does not vary with time. The clay GDS model also includes the ability to include vertical advective transport within the far field at 25%, 50%, 75%, and 100% of the domain width within the 20x20 node network. This allows for the simulation of fast paths that do not directly intersect the emplaced waste or the engineered barriers, but could degrade the isolation capability of the far field. The user is able to define the Darcy velocity in these fast paths along with a time and duration that the increased flow occurs. These could be used to evaluate the effects of increased flow, which could result from changes in regional recharge (or other processes) through high-level sensitivity studies.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.08.04	Effects of Repository Excavation on Flow Through the Host Rock	– Saturated flow (flow sink) – Unsaturated flow (capillary diversion, drift shadow) – Influx/Seepage into EBS (film flow, enhanced seepage [see also Influx/Seepage into EBS in 2.1.08.09]	No	It is assumed that there are no excavation effects on the host rock.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.08.05	Condensation Forms in Host Rock	– Condensation cap – Shedding [see also Thermal Effects on Flow in Geosphere in 2.2.11.01]	No	The conceptual model of a clay generic environment assumes it is fully saturated and isothermal (ambient temperature).	No	Condensation is not expected to form due to the high fluid pressures in the deep borehole disposal system.
2.2.08.06	Flow Through EDZ	– Saturated / Unsaturated flow – Fracture / Matrix flow	Yes	See FEP 2.2.01.01.	Partially	Disturbed rock zone (EDZ) does exist in the deep borehole. However, it is not explicitly modeled. It is coupled with the seal zone. Flow through the Seal Zone is implemented in \DBH_RN_transport\DBH_Transport_SealZone\SealZone_MultipleCells. Flow is modeled as fully saturated.
2.2.08.07	Mineralogic Dehydration	– Dehydration reactions release water and may lead to volume changes	Partially	Mineral dehydration effects are not explicitly considered. However, the user has the ability to change properties in the EDZ which could be used to evaluate the effects of mineral dehydration through high-level sensitivity studies.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.08.08	Groundwater Discharge to Biosphere Boundary	– Surface discharge (water table, capillary rise, surface water) – Flow across regulatory boundary	Partially	The Aquifer in the clay GDS model is represented as a swept away boundary condition to the far-field cell network. The radionuclide mass flux reaching the aquifer is used to determine the annual dose to the receptor. The mass flux for each radionuclide (g/yr) is multiplied by the specific activity (Bq/g) to determine the activity flux (Bq/yr) entering the aquifer. Dose conversion factors based on in the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.08.09	Groundwater Discharge to Well	– Human use (drinking water, bathing water, industrial) – Agricultural use (irrigation, animal watering)	Partially	The Aquifer in the clay GDS model is represented as a swept away boundary condition to the far-field cell network. The radionuclide mass flux reaching the aquifer is used to determine the annual dose to the receptor. The mass flux for each radionuclide (g/yr) is multiplied by the specific activity (Bq/g) to determine the activity flux (Bq/yr) entering the aquifer. Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose	Partially	The Biosphere is modeled using the IAEA's ERB 1B. ERB 1B is implemented at \DBH_Results\ERB1B_Biosphere_model.
2.2.09.00	2.09.CHEMICAL PROCESSES - CHEMISTRY					
2.2.09.01	Chemical Characteristics of Groundwater in Host Rock	– Water composition (radionuclides, dissolved species, …) – Water chemistry (temperature, pH, Eh, ionic strength …) – Reduction-oxidation potential – Reaction kinetics – Interaction with EBS – Interaction with host rock [see also Chemistry in Tunnels in 2.1.09.04, Chemical Interactions and Evolution in 2.2.09.03] [contributes to Chemistry of Water Flowing into Repository in 2.1.09.01]	Partially	The clay GDS model does not explicitly consider chemical characteristics of the ground water in the host rock. However, the user has the ability to define dissolved concentration limits and distribution coefficients. These are important parameters with respect to radionuclide transport that would be affected by chemical characteristics. The user's ability to change these parameters would allow for the assessment of chemical characteristics through high-level sensitivity studies.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.09.02	Chemical Characteristics of Groundwater in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Water composition (radionuclides, dissolved species, …) – Water chemistry (temperature, pH, Eh, ionic strength …) – Reduction-oxidation potential – Reaction kinetics - Interaction with other geologic units [see also Chemical Interactions and Evolution in 2.2.09.04]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	Partially	Solubility limits in the Upper Zone of the Borehole are defined at \Uncertain_Parameters\RN_Solubility and they are implemented at \DBH_RN_transport\DBH_Transport_UpperZone. Some radionuclides are modeled with unlimited solubility.
2.2.09.03	Chemical Interactions and Evolution of Groundwater in Host Rock	– Host rock composition and evolution (granite, clay, salt ...) – Evolution of water chemistry in host rock – Chemical effects on density – Interaction with EBS – Reaction kinetics – Mineral dissolution/precipitation – Redissolution of precipitates after dry-out [contributes to Chemistry in Host Rock in 2.2.09.01]	Partially	The clay GDS model does not explicitly consider chemical characteristics of the ground water in the host rock. However, the user has the ability to define dissolved concentration limits and distribution coefficients. These are important parameters with respect to radionuclide transport that would be affected by chemical characteristics. The user's ability to change these parameters would allow for the assessment of chemical characteristics through high-level sensitivity studies.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.09.04	Chemical Interactions and Evolution of Groundwater in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Host rock composition and evolution (granite, clay, salt ...) – Evolution of water chemistry in host rock – Chemical effects on density – Reaction kinetics – Mineral dissolution/precipitation – Recharge chemistry [contributes to Chemistry in Other Geologic Units in 2.2.09.02]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.05	Radionuclide Speciation and Solubility in Host Rock	– Dissolved concentration limits [controlled by Chemistry in Host Rock in 2.2.09.01]	Yes	Dissolved concentration limits are represented as log-triangular distributions with the parameters that define the distribution being user inputs. The sampled dissolved concentration limits are assumed not to vary with time and do not depend on the EBS environment (which is not explicitly modeled). The distribution parameters are input to the model in container:\Parameters_and_Materials\Input\Far_Field_Input The sampled values are determined in container :\Parameters_and_Materials\Epistemic_Parameters	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.09.06	Radionuclide Speciation and Solubility in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Dissolved concentration limits [controlled by Chemistry in Other Geologic Units in 2.2.09.02]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	Yes	Solubility limits in the Upper Zone of the Borehole are defined at \Uncertain_Parameters\RN_Solubility and they are implemented at \DBH_RN_transport\DBH_Transport_UpperZone. Some radionuclides are modeled with unlimited solubility.
2.2.09.50	2.09. CHEMICAL PROCESSES - TRANSPORT					
2.2.09.51	Advection of Dissolved Radionuclides in Host Rock	– Flow pathways and velocity – Advective properties (porosity, tortuosity) – Dispersion – Matrix diffusion – Saturation [see also Gas Phase Transport in 2.2.12.03]	Yes	The clay GDS model allows the user to define a vertical advective flow rate that does not vary with time. The clay GDS model also includes the ability to include vertical advective transport within the far field at 25%, 50%, 75%, and 100% of the domain width within the 20x20 node network. This allows for the simulation of fast paths that do not directly intersect the emplaced waste or the engineered barriers, but could degrade the isolation capability of the far field. The user is able to define the Darcy velocity in these fast paths along with a time and duration that the increased flow occurs.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.52	Advection of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Flow pathways and velocity – Advective properties (porosity, tortuosity) – Dispersion – Matrix diffusion – Saturation [see also Gas Phase Transport in 2.2.12.03]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	Partially	Advective transport of radionuclides through a saturated medium in the Upper Zone of the Borehole is implemented at \DBH_RN_transport\DBH_Transport_UpperZone\UpperBHZone_Pipe. Dispersion is also modeled. Matrix diffusion is not included in the model. For the purposes of FEP analysis the Upper Zone of the Borehole is being equated with the far-field Aquifer.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.09.53	Diffusion of Dissolved Radionuclides in Host Rock	– Gradients (concentration, chemical potential) – Diffusive properties (diffusion coefficients) – Flow pathways and velocity – Saturation	Yes	The far-field model includes the capability to represent either single-continuum radionuclide transport. The diffusive properties of the far-field (diffusive length, diffusive area, porosity, tortuosity) are user input parameters, entered from the input spreadsheet. These properties do not vary with time (static value) and are a combination of deterministic and stochastic parameters. The effective diffusion coefficient is determined from the free diffusion coefficient of water and the relative diffusivity of each element in water, which are user input values from the input spreadsheet. These are input to the model in container :\Parameters_and_Materials\Input\Free_Diffusion	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.54	Diffusion of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Gradients (concentration, chemical potential) – Diffusive properties (diffusion coefficients) – Flow pathways and velocity – Saturation	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	Yes	Diffusive transport of radionuclides through a saturated medium in the Upper Zone of the Borehole is implemented at \DBH_RN_transport\DBH_Transport_UpperZone\UpperBHZone_Pipe. For the purposes of FEP analysis the Upper Zone of the Borehole is being equated with the far-field Aquifer.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.09.55	Sorption of Dissolved Radionuclides in Host Rock	– Surface complexation properties – Flow pathways and velocity – Saturation [see also Chemistry in Host Rock in 2.2.09.01]	Yes	Distribution coefficients (reversible sorption) are represented as log-triangular distributions with the parameters that define the distribution being user inputs. The sampled distribution coefficients are assumed not to vary with time and do not depend on the far-field environment (which is not explicitly modeled). Containers where input is defined is :\Parameters_and_Materials\Input\Far_Field_Input Stochastic parameters are sampled in container :\Parameters_and_Materials\Epistemic_Parameters	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.56	Sorption of Dissolved Radionuclides in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Surface complexation properties – Flow pathways and velocity – Saturation [see also Chemistry in Host Rock in 2.2.09.01]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	Yes	Sorption coefficients for the Upper Zone of the Borehole are defined at \Uncertain_Parameters\DBH_transport_Parameters\DBH_Kd_data\DBH_Kd_UpperZone and they are implemented at \DBH_RN_transport\DBH_Transport_UpperZone. Some radionuclides are modeled with sorption coefficients set equal to zero.
2.2.09.57	Complexation in Host Rock	– Presence of organic complexants (humates, fulvates, carbonates, …) – Enhanced transport of radionuclides associated with organic complexants [see Radionuclide Speciation in 2.2.09.05 for inorganic complexation]	No	It was assumed that no organic complexation would occur in the host rock.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.09.58	Complexation in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Presence of organic complexants (humates, fulvates, carbonates, …) – Enhanced transport of radionuclides associated with organic complexants [see Radionuclide Speciation in 2.2.09.06 for inorganic complexants]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.59	Colloidal Transport in Host Rock	– Flow pathways and velocity – Saturation – Advection – Dispersion – Diffusion – Sorption – Colloid concentration	No	Colloidal radionuclide transport was not considered in this version of the clay GDS model	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.60	Colloidal Transport in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	– Flow pathways and velocity – Saturation – Advection – Dispersion – Diffusion – Sorption – Colloid concentration	No	Colloidal radionuclide transport was not considered in this version of the clay GDS model	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.09.61	Radionuclide Transport Through EDZ	– Advection – Dispersion – Diffusion – Sorption	Yes	See FEP 2.2.01.01	Partially	Disturbed rock zone (EDZ) does exist in the deep borehole. However, it is not explicitly modeled. It is coupled with the seal zone. Flow through the Seal Zone is implemented in \DBH_RN_transport\DBH_Transport_SealZone\SealZone_MultipleCells. Advective and diffusive transport is modeled through the bentonite of the Seal Zone. Sorption coefficients for the Seal Zone are defined at \Uncertain_Parameters\DBH_transport_Parameters\DBH_Kd_data\DBH_Kd_SealZone and they are implemented at \DBH_RN_transport\DBH_Transport_SealZone. Some radionuclides are modeled with sorption coefficients set equal to zero.
2.2.09.62	Dilution of Radionuclides in Groundwater – Host Rock – Other Geologic Units	– Mixing with uncontaminated groundwater – Mixing at withdrawal well [see also Groundwater Discharge to Well in 2.2.08.09]	Partially	The clay GDS model allows the user to define, from the input spreadsheet, a dilution factor.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.63	Dilution of Radionuclides with Stable Isotopes – Host Rock – Other Geologic Units	– Mixing with stable and/or naturally occurring isotopes of the same element	No	It is assumed that no dilution with stable isotopes occurs.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.2.09.64	Radionuclide Release from Host Rock – Dissolved – Colloidal – Gas Phase	– 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) [contributions from Dissolved in 2.2.09.51/53/55, Colloidal in 2.2.09.59, Gas Phase in 2.2.12.03, EDZ in 2.2.09.61]	Yes	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.09.65	Radionuclide Release from Other Geologic Units – Dissolved – Colloidal – Gas Phase	– Spatial and temporal distribution of releases to the Biosphere (due to varying flow pathways and velocities, varying transport properties) [see also Groundwater Discharge to Biosphere Boundary in 2.2.08.08, Groundwater Discharge to Well in 2.2.08.09, Recycling of Accumulated Radionuclides in 2.3.09.55] [contributions from Dissolved in 2.2.09.52/54/56, Colloidal in 2.2.09.60, Gas Phase in 2.2.12.03]	No	Due to the generic nature of the clay GDS model, additional geologic units are not considered. The clay GDS model assumes that there is an aquifer immediately above the clay formation and applies a swept-away (zero concentration) boundary condition.	Yes	The release of radionuclides from the Upper Zone of the Borehole is implemented at \DBH_RN_transport\DBH_Transport_UpperZone\UpperBHZone_Pipe. Documents the mass flux of individual radionuclides as a function of time at the top of the Upper Zone of the Borehole.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.10.00	2.10. BIOLOGICAL PROCESSES					
2.2.10.01	Microbial Activity in Host Rock	Formation of complexants – Formation and stability of microbial colloids – Biodegradation – Bioaccumulation [see also Complexation in Host Rock in 2.2.09.57]	No	Microbial activity in the geosphere is not considered.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.10.02	Microbial Activity in Other Geologic Units (Non-Host-Rock) – Confining units – Aquifers	Formation of complexants – Formation and stability of microbial colloids – Biodegradation – Bioaccumulation [see also Complexation in Other Geologic Units in 2.2.09.58]	No	Microbial activity in the geosphere is not considered.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.11.00	2.11. THERMAL PROCESSES					
2.2.11.01	Thermal Effects on Flow in Geosphere – Repository-Induced – Natural Geothermal	– Altered saturation / relative humidity (dry-out, resaturation) – Altered gradients, density, and/or flow pathways – Vapor flow – Condensation	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	Partially	Heat generation in the disposal zone and associated thermal-hydrologic effects are explicitly modeled in a 3D process model. However, only the resulting vertical ground water fluxes through the borehole are used in the GDS model.
2.2.11.02	Thermally-Driven Flow (Convection) in Geosphere	– Convection	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.11.03	Thermally-Driven Buoyant Flow / Heat Pipes in Geosphere	– Vapor flow	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	Partially	Heat generation in the disposal zone and associated thermal-hydrologic effects are explicitly modeled in a 3D process model. However, only the resulting vertical ground water fluxes through the borehole are used in the GDS model. Heat pipes are not included.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.2.11.04	Thermal Effects on Chemistry and Microbial Activity in Geosphere	– Mineral precipitation / dissolution – Altered solubility [contributes to Chemistry in 2.2.09.01 and 2.2.09.02]	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.11.05	Thermal Effects on Transport in Geosphere	– Thermal diffusion (Soret effect) – Thermal osmosis	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.11.06	Thermal-Mechanical Effects on Geosphere	– Thermal expansion / compression – Altered properties of fractures, faults, rock matrix	No	At present, a constant temperature of 25°C is assumed. At some point in the future, various thermal processes will be considered for possible inclusion in the GPAM.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
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)	No	Thermal processes within the EBS are not considered. A constant ambient temperature of 25°C is assumed.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.12.00	2.12. GAS SOURCES AND EFFECTS					
2.2.12.01	Gas Generation in Geosphere	– Degassing (clathrates, deep gases) – Microbial degradation of organics – Vaporization of water	No	Gas generation and its effect on the geosphere are not included in the model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
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 [see also Buoyant Flow/Heat Pipes in 2.2.11.03]	No	Gas generation and its effect on the geosphere are not included in the model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.12.03	Gas Transport in Geosphere	– Gas phase transport – Gas phase release from Geosphere	No	Gas generation and its effect on the geosphere are not included in the model.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.2.14.00	2.14. NUCLEAR CRITICALITY					
2.2.14.01	Criticality in Far-Field	– Formation of critical configuration	No	Far-field criticality is not included in the model. Criticality in the far field is not expected.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.00.00	3. SURFACE ENVIRONMENT					
2.3.01.00	3.01. SURFACE CHARACTERISTICS					
2.3.01.01	Topography and Surface Morphology	– Recharge and discharge areas	No	The conceptual model of a clay generic environment assumes sufficient isolation from surface topography or morphology effects. Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.02.01	Surficial Soil Type	– Physical and chemical attributes	No	The conceptual model of a clay generic environment assumes sufficient isolation from surface soils. Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.3.04.01	Surface Water	– Lakes, rivers, springs – Dams, reservoirs, canals, pipelines – Coastal and marine features – Water management activities	No	The Aquifer in the clay GDS model is represented as a swept away boundary condition to the far-field cell network. The radionuclide mass flux reaching the aquifer is used to determine the annual dose to the receptor. The mass flux for each radionuclide (g/yr) is multiplied by the specific activity (Bq/g) to determine the activity flux (Bq/yr) entering the aquifer. Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.05.01	Biosphere Characteristics	– Climate – Soils – Flora and fauna – Microbes – Evolution of biosphere (natural, anthropogenic – e.g., acid rain) [see also Climate Change in 1.3.01.01, Surficial Soil Type in 2.3.02.01, Microbial Activity in 2.3.10.01]	Partially	The Aquifer in the clay GDS model is represented as a swept away boundary condition to the far-field cell network. The radionuclide mass flux reaching the aquifer is used to determine the annual dose to the receptor. The mass flux for each radionuclide (g/yr) is multiplied by the specific activity (Bq/g) to determine the activity flux (Bq/yr) entering the aquifer. Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	Partially	The Biosphere is modeled using the IAEA's ERB 1B. ERB 1B is implemented at \DBH_Results\ERB1B_Biosphere_model.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.3.07.00	3.07. MECHANICAL PROCESSES					
2.3.07.01	Erosion	– Weathering – Denudation – Subsidence [see also Subsidence in 1.2.02.01, Periglacial Effects in 1.3.04.01, Glacial Effects in 1.3.05.01, Surface Runoff in 2.3.08.02, and Soil and Sediment Transport in 2.3.09.53]	No	The conceptual model of a clay generic environment assumes sufficient isolation from surface erosion effects.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.07.02	Deposition	– Weathering	No	The conceptual model of a clay generic environment assumes sufficient isolation from weathering effects.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.07.03	Animal Intrusion into Repository		No	The conceptual model of a clay generic environment assumes sufficient isolation from animal intrusion effects.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.3.08.00	3.08. HYDROLOGIC PROCESSES					
2.3.08.01	Precipitation	– Spatial and temporal distribution [see also Climate Change in 1.3.01.01] [contributes to Infiltration in 2.3.08.03]	No	The conceptual model of a clay generic environment assumes sufficient isolation from surface hydrologic effects. The Aquifer in the clay GDS model is represented as a swept away boundary condition to the far-field cell network. The radionuclide mass flux reaching the aquifer is used to determine the annual dose to the receptor. The mass flux for each radionuclide (g/yr) is multiplied by the specific activity (Bq/g) to determine the activity flux (Bq/yr) entering the aquifer. Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.3.08.02	Surface Runoff and Evapotranspiration	– Runoff, impoundments, flooding, increased recharge – Evaporation – Condensation – Transpiration (root uptake) [see also Climate Change in 1.3.01.01, Erosion in 2.3.07.01] [contributes to Infiltration in 2.3.08.03]	No	The conceptual model of a clay generic environment assumes sufficient isolation from surface hydrologic effects. The Aquifer in the clay GDS model is represented as a swept away boundary condition to the far-field cell network. The radionuclide mass flux reaching the aquifer is used to determine the annual dose to the receptor. The mass flux for each radionuclide (g/yr) is multiplied by the specific activity (Bq/g) to determine the activity flux (Bq/yr) entering the aquifer. Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.3.08.03	Infiltration and Recharge	– Spatial and temporal distribution – Effect on hydraulic gradient – Effect on water table elevation [see also Topography in 2.3.01.01, Surficial Soil Type in 2.3.02.01] [contributes to Effects of Recharge in 2.2.08.03]	No	The conceptual model of a clay generic environment assumes sufficient isolation from surface hydrologic effects. The Aquifer in the clay GDS model is represented as a swept away boundary condition to the far-field cell network. The radionuclide mass flux reaching the aquifer is used to determine the annual dose to the receptor. The mass flux for each radionuclide (g/yr) is multiplied by the specific activity (Bq/g) to determine the activity flux (Bq/yr) entering the aquifer. Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.3.09.00	3.09. CHEMICAL PROCESSES - CHEMISTRY					
2.3.09.01	Chemical Characteristics of Soil and Surface Water	– Altered recharge chemistry (natural) – Altered recharge chemistry (anthropogenic – e.g., acid rain) [contributes to Chemical Evolution of Groundwater in 2.2.09.04]	No	The conceptual model of a clay generic environment assumes sufficient isolation from surface chemical processes. The Aquifer in the clay GDS model is represented as a swept away boundary condition to the far-field cell network. The radionuclide mass flux reaching the aquifer is used to determine the annual dose to the receptor. The mass flux for each radionuclide (g/yr) is multiplied by the specific activity (Bq/g) to determine the activity flux (Bq/yr) entering the aquifer. Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.02	Radionuclide Speciation and Solubility in Biosphere	– Dissolved concentration limits	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.03	Radionuclide Alteration in Biosphere	– Altered physical and chemical properties – Isotopic dilution	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.50	3.09. CHEMICAL PROCESSES - TRANSPORT					
2.3.09.51	Atmospheric Transport Through Biosphere	– Radionuclide transport in air, gas, vapor, particulates, aerosols – Processes include: wind, plowing, degassing, precipitation	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
2.3.09.52	Surface Water Transport Through Biosphere	– Radionuclide transport and mixing in surface water – Processes include: lake mixing, river flow, spring discharge, overland flow, irrigation, aeration, sedimentation, dilution [see also Surface Water in 2.3.04.01]	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.53	Soil and Sediment Transport Through Biosphere	– Radionuclide transport in or on soil and sediments – Processes include: fluvial (runoff, river flow), eolian (wind), saltation, glaciation, bioturbation (animals) [see also Erosion in 2.3.07.01, Deposition in 2.3.07.02	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.54	Radionuclide Accumulation in Soils	– Leaching/evaporation from discharge (well, groundwater upwelling) – Deposition from atmosphere or water (irrigation, runoff)	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.09.55	Recycling of Accumulated Radionuclides from Soils to Groundwater	[see also Radionuclide Release in 2.2.09.65]	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.3.10.00	3.10. BIOLOGICAL PROCESSES					
2.3.10.01	Microbial Activity in Biosphere	– Effect on biosphere characteristics – Effect on transport through biosphere	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.3.11.00	3.11. THERMAL PROCESSES					
2.3.11.01	Effects of Repository Heat on Biosphere		No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.4.00.00	4. HUMAN BEHAVIOR					
2.4.01.00	4.01. HUMAN CHARACTERISTICS					
2.4.01.01	Human Characteristics	– Physiology – Metabolism – Adults, children [contributes to Radiological Toxicity in 3.3.06.02]	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.4.01.02	Human Evolution	– Changing human characteristics – Sensitization to radiation – Changing lifestyle	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
2.4.04.00	4.04. LIFESTYLE					
2.4.04.01	Human Lifestyle	– Diet and fluid intake (food, water, tobacco/drugs, etc.) – Dwellings – Household activities – Leisure activities [see also Land and Water Use in 2.4.08.01] [contributes to Ingestion in 3.3.04.01, Inhalation in 3.3.04.02, External Exposure in 3.3.04.03]	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.4.08.00	4.08. LAND AND WATER USE					
2.4.08.01	Land and Water Use	– Agricultural (irrigation, plowing, fertilization, crop storage, greenhouses, hydroponics) – Farms and Fisheries (feed, water, soil) – Urban / Industrial (development, energy production, earthworks, population density) – Natural / Wild (grasslands, forests, bush, surface water)	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
2.4.08.02	Evolution of Land and Water Use	– New practices (agricultural, farming, fisheries) – Technological developments – Social developments (new/expanded communities)	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
3.0.00.00	3. RADIONUCLIDE / CONTAMINANT FACTORS (BIOSPHERE)					
3.1.00.00	1. CONTAMINANT CHARACTERISTICS					
3.2.00.00	2. RELEASE / MIGRATION FACTORS					
3.3.00.00	3. EXPOSURE FACTORS					
3.3.01.00	3.01. RADIONUCLIDE / CONTAMINANT CONCENTRATIONS					
3.3.01.01	Radionuclides in Biosphere Media	– Soil – Surface Water – Air – Plant Uptake – Animal (Livestock, Fish) Uptake – Bioaccumulation [contributions from Radionuclide Release from Geologic Units in 2.2.09.65, Transport Through Biosphere in 2.3.09.51/52/53/54/55]	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
3.3.01.02	Radionuclides in Food Products	– Diet and fluid sources (location, degree of contamination, dilution with uncontaminated sources) – Foodstuff and fluid processing and preparation (water filtration, cooking techniques) [see also Land and Water Use in 2.4.08.01, Radionuclides in Biosphere Media in 3.3.01.01]	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	UFD FEP Title	Process/Issue Description	Yes Partially No	Discussion	Yes Partially No	Discussion
3.3.01.03	Radionuclides in Non-Food Products	– Dwellings (location, building materials and sources, fuel sources) – Household products (clothing and sources, furniture and sources, tobacco, pets) – Biosphere media [see also Land and Water Use in 2.4.08.01, Radionuclides in Biosphere Media in 3.3.01.01]	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
3.3.04.00	3.04. EXPOSURE MODES					
3.3.04.01	Ingestion	– Food products – Soil, surface water	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
3.3.04.02	Inhalation	– Gases and vapors – Suspended particulates (dust, smoke, pollen)	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
3.3.04.03	External Exposure	– Non-Food products – Soil, surface water	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Table B-2. FEPs Mapping of the Clay and Deep Borehole GDS Models (continued)

FEP Information			Capability Included in Clay/Shale GDS Model		Capability Included in Deep Borehole GDS Model	
UFD FEP ID	**UFD FEP Title**	**Process/Issue Description**	**Yes Partially No**	**Discussion**	**Yes Partially No**	**Discussion**
3.3.06.00	3.06. TOXICITY / EFFECTS					
3.3.06.01	Radiation Doses	– Exposure rates (ingestion, inhalation, external exposure) – Dose conversion factors – Gases and vapors – Suspended particulates (dust, smoke, pollen)	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	Partially	The ERB 1B dose conversion factors are used in the Biosphere Model. They are implemented at \DBH_Results\ERB1B_Biosphere_model.
3.3.06.02	Radiological Toxicity and Effects	– Human health effects from radiation doses	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.
3.3.06.03	Non-Radiological Toxicity and Effects	– Human health effects from non-radiological toxicity	No	Dose conversion factors based on the IAEA's BIOMASS dose model for a simple drinking water well pathway (ERB 1B) were used to convert the mass flux to annual dose.	No	There are no near-term plans to include this FEP. Model development is at too early a stage to consider inclusion.

Appendix C

Solubility and Equilibrium Linear Sorption Coefficient for Some Radionuclides

C-1. Solubility and Equilibrium Linear Sorption Coefficient for Some Radionuclides

This memo documents initial preliminary estimates of the solubility and equilibrium linear sorption coefficient of some minor radionuclides in the disposal zone of a generic deep borehole repository. These estimates are also used in a generic salt repository as it is appropriate. It is emphasized that these values in the table below are estimates made in the absence of much-needed thermodynamic data. No activity coefficient corrections were made to all solubility estimates. Improvements to the estimates will be made in a future iteration.

Table C-1. Preliminary Estimates of Solubility and Equilibrium Linear Sorption Coefficient for Selected Radionuclides

Element	Solubility (mol/L)	Kd (mL/g)
Zr	10^{-10}	1000
Se	~ $10^{-4.7}$	50
Pd	$10^{-3.4}$	100
Sn	$10^{-3.8}$	20
Nb	$10^{-4.8}$	10
Cl	4.2	0
Sb	$10^{-4.2}$	100

- Zr—Constrained by the ZrO_2 solubility at pH 8.5 and 25°C (Baes and Mesmer, 1979). K_d values were ball-parked from the low temperature data by McKinley and Scholtis (1992).
- *Se*—Constrained by the Fe-Se solubility-limiting phase using the 60°C data from Iida et al. (2007) and the following website:

  http://www.google.com/url?sa=t&source=web&cd=2&sqi=2&ved=0CBoQFjAB&url=http%3A%2F%2Fmofap07.in2p3.fr%2F18janvier%2Fiida.pdf&rct=j&q=Selenium%20solubility%2025%20C&ei=V5ncTID1JlfvsgbJ84GiBA&usg=AFQjCNFb8atb1mUiHZp40kViEQZdnQ59mA&cad=rja.

  K_d values were ball-parked from the low temperature data by McKinley and Scholtis (1992).
- *Pd*—The solubility value was obtained from a bounding PHREEQC calculation at 200°C assuming that PdO controls solubility. K_d values were obtained from analogy with other divalent cations.
- *Sn*—The solubility value was obtained from PHREEQC calculations with assumed SnO saturation and pH 8.5 at 200°C. K_d values were ball-parked from the low temperature data by McKinley and Scholtis (1992).

- *Nb*—Very little data is available for Nb solubility. The solubility value in the table is based on the solubility measurement at 19°C. K_d values were ball-parked from the low temperature values for Sr, another divalent cation, by McKinley and Scholtis (1992).
- *Cl*—The solubility value is based on halite saturation at 200°C and an equimolar amount of Na^+.
- *Sb*—Based on the data at 25°C by Baes and Mesmer (1979). There is data in the hydrothermal ore literature, but analysis has not been completed. A bounding PHREEQC calculation indicates that the solubility value in the table is in the ball-park. There is no K_d data reported, so the low end Kd value for Am, uncharged, hydrolyzed trivalent cation, is used.