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SOAR: A MODEL FOR SCOPING OF OPTIONS AND ANALYZING RISK VERSION 1.0 USER GUIDE

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Prepared by

Chris Markley,[1] Osvaldo Pensado,[2] Jin-Ping Gwo,[1] James Winterle,[2] Tae Ahn,[1] Roland Benke,[2] Tianqing Cao,[1] Hipólito González,[1] Anita Gray,[1] Xihua He,[2] Ronald Janetzke,[2] Hundal Jung,[2] Greg Oberson,[1] Pavan Shukla,[2] Timothy Sippel,[1] Stuart Stothoff,[2] and Lynn Tipton[2]

[1]U.S. Nuclear Regulatory Commission
Washington, DC

[2]Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

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EXECUTIVE SUMMARY

This user guide describes the operation and capabilities of the Scoping of Options and Analyzing Risk (SOAR) model. The SOAR model is designed to provide the U.S. Nuclear Regulatory Commission (NRC) staff timely risk and performance insights for a variety of potential high-level radioactive waste (HLW) disposal options. NRC staff developed SOAR with the assistance of its contractor, the Center for Nuclear Waste Regulatory Analyses. The model applies technical knowledge developed over more than two decades in the field of nuclear waste repository performance assessment modeling. This manual describes the capabilities, limitations, computational approaches, parameters, and operation of the SOAR model.

Public acceptance of any HLW disposal site cannot be achieved without technical and ethical trust in its regulators. Similarly, expenditure of public funds must be carefully evaluated to ensure effectiveness and efficiency in the regulatory process. This model is one of the elements identified in NRC's Plan for Integrating Spent Nuclear Fuel Regulatory Activities (NRC, 2010) that focuses on achieving a predictable, effective, and efficient regulatory program. The SOAR model is an analytic scoping tool that the staff will use to develop an effective and efficient risk-informed, performance-based licensing program for geologic disposal of HLW. The short-term programmatic needs include, but are not limited to (i) effectively and efficiently adapting the regulatory process to changes in the national policy on high-level disposal; (ii) responding to inquiries from Congress, the Commission, the public, and the U.S. Department of Energy's Blue Ribbon Commission; (iii) preliminary identification of potential risk and performance insights for a range of geologic disposal options for HLW (e.g., granite, clay, porous media); and (iv) identifying future analytic and experimental activities needed to develop rigorous independent confirmatory capabilities to meet NRC's statutory responsibilities. The long-term programmatic needs include the development of an independent, confirmatory, analytic capability to assist licensing reviews, for which this model is a preliminary component. The SOAR model is not intended to be used as a licensing tool. The SOAR model is only one element of NRC's Plan for Integrating Spent Nuclear Fuel Regulatory Activities. It is a technical starting point from which an effective and efficient regulatory program will be developed for future licensing applications.

Reference

NRC. "Plan for Integrating Spent Nuclear Fuel Regulatory Activities." ML1012410380. Washington, DC: NRC. 2010

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT DATA

DATA: The **S**coping of **O**ptions and **A**nalyzing **R**isk (SOAR) model was developed outside a formal quality control program for software development [CNWRA Technical Operating Procedure (TOP)–18]. However, simplified procedures (mutually agreed upon by NRC and CNWRA staffs) were implemented for model development that included version control and verification testing. Some input data to SOAR documented in this report are primarily experimental observations obtained from other publicly available sources. Each data source is cited in this report and should be consulted for determining the level of quality for those cited data. Scientific Notebooks 1038E (Stothoff, 2010) and 1036E (Tipton, 2010) document SOAR model development in work areas related to the waste form and near-field modules.

ANALYSES AND CODES: SOAR was developed using GoldSim (GoldSim Technology Group, LLC, 2010). As previously stated, SOAR development did not follow TOP–18, but a simplified procedure for version control and software verification. The SOAR model utilizes the Microsoft® Access® Database (Microsoft Corporation, 2007a) for database management. Inventory calculations used as input to SOAR were performed using the ORIGEN-ARP (Gauld, et al., 2009) component of the SCALE6 code system (ORNL, 2009).

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1 INTRODUCTION

1.1 What Is a Performance Assessment?

With respect to the long-term disposition of high-level radioactive waste (HLW) in a geologic disposal system, a performance assessment is a systematic analysis that quantifies the risk triplet questions

- What can happen?
- How likely is it?
- What are the consequences?

In general, a performance assessment

- Identifies the features, events, processes, and sequences of events and processes that might affect the geologic disposal system and their probabilities of occurring

- Examines the effects of those features, events, processes, and sequences of events and processes upon the performance of the geologic disposal system

- Estimates some quantitative performance metric, weighted by its probability of occurrence, be it a dose to a receptor or radionuclide releases

Because geologic disposal systems are relatively large in both spatial and temporal scales, development of a performance assessment model can be a complex process. From a regulatory perspective, an initial performance assessment is developed in four steps:

(1) Identify the geologic disposal system to be assessed, and conduct a scenario analysis to develop a conceptual model of the geologic disposal system including the approach to evaluate the uncertainties.

(2) Develop an initial model, appropriate for use in scoping activities, to determine features, events, or processes that may be of risk or performance significance.

(3) Refine the performance assessment until it is adequate for the intended use to risk inform regulation development. Features, events, and processes may be added or removed in this step.

(4) Analyze the results to provide risk insights when developing risk-informed and performance-based regulatory programs.

Additional data collection and analysis, including the potential development of more detailed process models in support of site-specific evaluations, will often result in iteration of steps 3 and 4. Based on the current uncertainty in the national policy for HLW disposal, the performance assessment model described in this user guide is generic in nature and not designed for use as a detailed site-specific evaluation. This model is intended to be used as a tool for scoping assessments when developing an effective and efficient risk-informed and performance-based regulatory program.

1.2 Purpose of the Scoping of Options and Analyzing Risk Model

The U.S. Nuclear Regulatory Commission (NRC) has developed a performance assessment model named Scoping of Options and Analyzing Risk (SOAR). This model is one of the elements identified in NRC's Plan for Integrating Spent Nuclear Fuel Regulatory Activities (NRC, 2010) that focuses on achieving a predictable, effective, and efficient regulatory program.

The model described herein is a starting point for a tool that will ultimately provide the NRC staff timely risk and performance insights for a variety of potential HLW disposal options. These insights will support development of a regulatory framework in an evolving regulatory environment for licensing and regulating permanent disposal of HLW. The model is based on relatively simple or generic representations of features, events, and processes that can be parameterized or modified to allow flexibility to consider a variety of alternative waste form characteristics; engineered barrier materials; and geologic, hydrologic, and geochemical settings. Additional complexity may be added to model components in the future that represent specific site characteristics or processes not considered in this initial version. Due to the abstracted representation of features, events, and processes, application and results from the current version of the SOAR model are intended to be applied for scoping analyses and should be used with caution. Some specific limitations of SOAR are discussed in Section 2.2.2.

Considering the current uncertainty in the U.S. national policy for HLW disposal, the SOAR model presented in this report is designed with the goal of maximizing flexibility to consider a variety of disposal options. The simplified model abstractions and associated parameter inputs are built upon the knowledge and experience gained by the NRC staff and the Center for Nuclear Waste Regulatory Analyses, and from other domestic and international performance assessments for a variety of geologic disposal options. The model is parameterized with data available in existing literature from international disposal programs for a variety of engineered and geologic materials. The default parameter distributions and preliminary technical bases are listed in Appendix A, and their use in the model calculations is detailed throughout Chapter 4. Many of the input parameters are stochastically sampled from broad ranges of values to account for uncertainty and variability. This stochastic sampling approach permits use of model results to evaluate parameter uncertainties that have the potential to affect radionuclide release and receptor dose. The insights gained from analyses with the SOAR model will be used to assist the NRC staff to focus its evolving regulatory program for HLW disposal on characteristics of geologic disposal important to waste isolation. The model will also assist the staff in identifying regulatory research and development activities related to physical processes (e.g., radionuclide solubility, water flow) and characteristics (e.g., waste package materials, waste form inventories and characteristics, host-rock types) on which a regulatory program should focus.

The detailed analytic methods, abstraction models, and input parameters used in SOAR will continue to be developed as the U.S. national policy evolves and potential options for waste form characteristics and ultimate disposal options become more clear and site specific. As candidate sites or conceptual approaches are identified, each will require an analysis of site-specific features, events, and processes that may necessitate different calculations for risk assessment. Accordingly, the modular structure and analytic approach of the model are designed to accommodate additional complexity and more detailed process-level models in future revisions.

1.3 Objectives

The objectives of the SOAR model are to

- Provide a foundation for developing analytic capabilities that assist the NRC staff to develop an effective and efficient regulatory program for reviewing and licensing a disposal site in any geologic medium

- Enhance the NRC staff's technical capabilities by creating a model in a visual-based software environment [GoldSim™ (registered trademark of GoldSim Technology Group, LLC)] that promotes model transparency

- Develop a flexible scoping tool to provide initial risk and performance insights of a wide variety of HLW disposal options

- Develop an efficient computational tool for future expansion or implementation of alternative approaches

As indicated previously, flexibility is a key element in several of the model objectives. A detailed discussion of how flexibility is built into the model is provided in Section 3.2.

The objectives of this SOAR User Guide are to

- Provide an overview of the bases, equations, input, output, and assumptions

- Provide an overview of the modeling environment, key flexibilities, and general guidance for using the model

- Provide an overview of the key aspects of the model components

- Summarize activities conducted to provide confidence in SOAR results

2 OVERVIEW OF SCOPING OF OPTIONS AND ANALYZING RISK

2.1 Contents of Scoping of Options and Analyzing Risk

2.1.1 System Overview

The Scoping of Options and Analyzing Risk (SOAR) model approximates performance of a hypothetical geologic nuclear waste disposal system. Figure 2-1 illustrates the general conceptual model considered in (SOAR). The engineered portion of the system comprises waste form, waste package, and engineered backfill material which is contained within the near-field. The natural subsystem is modeled by the far-field. The waste form may consist of different masses of (i) commercial spent nuclear fuel (SNF), (ii) high-level waste glass (HLWg), (iii) high-level waste ceramic (HLWc), and (iv) spent mixed-oxide (sMOX) fuel waste forms, which degrade at different rates. Failure of waste packages is implemented as gradual failure over time (i.e., distributed failure) and instantaneous failure of a given number of waste packages at specified times (i.e., stepwise failure). These two failure abstractions allow flexibility to represent different waste package materials and failure mechanisms. Three additional user-defined waste package failure abstractions are also available and may be used to represent various disruptive events (Disruptive Events model component). Radionuclides released from degraded waste forms migrate out of the waste package, through a backfill region, and into the surrounding natural system. The natural system is represented by three "legs" with characteristics specified to represent transport pathways through up to three geologic media. The user can define the length of each transport leg. Radionuclide transport through each leg can be either through porous rock; fractured, low-permeability rock; or unconsolidated sediments. The inset in Figure 2-1 indicates that the conceptual model for radionuclide release and transport need not be constrained to a horizontal system layout. Modeled radionuclide releases from the natural system are used to assess the performance of a system as a whole. Performance metrics include cumulative radionuclide release and annual dose to receptors from drinking water.

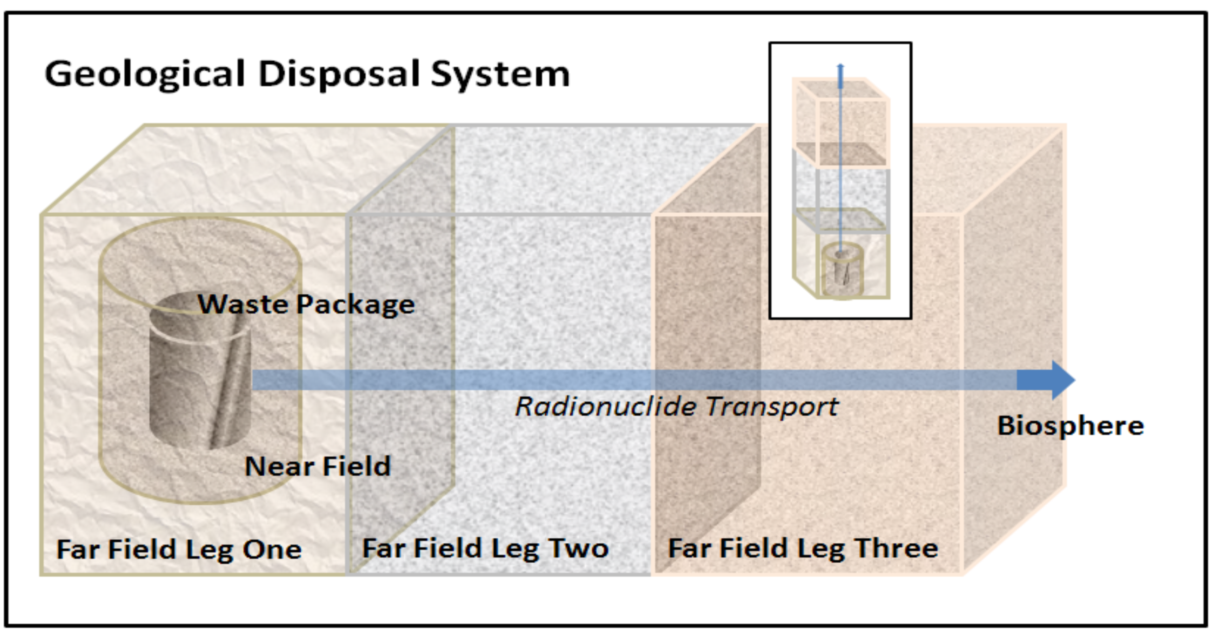

Figure 2-1. Schematic Illustration of Disposal System Modeled in SOAR

2.1.2 Component Overviews

The main model components of the SOAR model are

- Waste Form
- Waste Package
- Near Field (engineered and disturbed zones)
- Far Field (natural system)
- Biosphere

A secondary model component is Disruptive Events, which complements the Waste Package model component to consider a range of processes that could cause waste package breach. These model components are briefly described in the following paragraphs. More detailed descriptions of the computational approaches and input parameters for each of the five model components are presented in Chapter 4. Chapter 4 also includes an overview of the Disruptive Events abstraction implemented in SOAR.

The SOAR Waste Form model component includes up to four types of waste forms

- Commercial SNF
- HLWg
- HLWc
- sMOX fuel

The user can define the total inventory and relative amounts of each waste form. Both matrix-bound and unbound radionuclide inventories can be considered and may be released from a waste package after a breach. Matrix-bound radionuclides are those that are embedded in a waste form matrix (e.g., glass, SNF matrix) and are released at a rate controlled by the rate of waste form matrix degradation. Unbound radionuclides are not embedded in the waste form matrix or loosely bound (e.g., radionuclides accumulated in waste form grain boundaries, or in the gap between spent fuel and cladding), and are assumed instantly released after breach of the waste package and contact with groundwater. Waste form degradation is assumed to occur at a constant rate, calculated based on the type of waste form and chemical environment.

The Waste Package model component includes two modes of waste package failure. The first mode considers failures distributed over time (e.g., uniform or normal distribution of waste package failure with respect to time). This time-distributed failure mechanism is used to approximate general (uniform) corrosion that progresses slowly over time, with varying corrosion rates from waste package to waste package, causing waste packages to fail at different times. The second failure mechanism implements failures as a step function (e.g., 10 percent of waste packages fail at a specific time). This failure mechanism is used to approximate localized corrosion, which affects passive metals such as stainless steel, but progresses relatively fast when it occurs. The timing, number of failures, and breach area are computed based on the waste package material selected and stochastically sampled input parameters, for example, generalized corrosion rates. With appropriately modified inputs, the time of failure and breach area could be adapted to approximate other failure mechanisms, such as stress corrosion cracking and mechanical damage.

The Near Field model component includes advective and diffusive radionuclide releases through a breach in the waste package, a surrounding diffusive barrier, and a zone of surrounding host rock connected to a flow path in the Far Field. The diffusive barrier is used to represent engineered backfill, and the user can specify its presence or absence.

The Far Field model component accounts for radionuclide transport through groundwater pathways in the natural system. The term "far field" refers to radionuclide transport in a region far from the engineered and disturbed zones represented in the Near Field model component. The Far Field model component is divided into three distinct zones, referred to as transport legs, used to represent the potential transition of groundwater pathways through different geologic environments. Each of the three transport legs can be specified to be either fracture-dominated (e.g., granite rock) or matrix-dominated (e.g., clay, alluvium) transport pathways. The user can define the length of each transport leg.

The Biosphere model component is used for the computation of doses to a hypothetical receptor that drinks groundwater from a well that captures radionuclides at the end of the Far Field transport pathway. The current model component only calculates ingestion doses from contaminated drinking water.

2.2 Model Development and Status

2.2.1 Model Conceptualization Process

Performance assessment models are usually based upon a detailed scenario analysis for a specific location. Because SOAR is a scoping tool to support regulatory programs that incorporate performance and risk insights in a variety of potential disposal systems, a detailed scenario analysis was not conducted. Rather, the general conceptual approach described in Section 2.1 was developed to allow flexibility to consider a variety of engineered and natural system features and processes.

2.2.2 Model Limitations

Comparison of the SOAR model to the Nuclear Energy Agency (NEA, 2006) features, events, and processes list identified certain features, events, and processes that are not explicitly included in the model. Exclusion of certain features, events, and processes from this initial version of the model was simply done to accelerate model development. The model retains flexibility to consider additional features, events, and processes in future versions. The following potentially significant processes are not currently included in the initial version of the SOAR model:

- The SOAR model does not explicitly consider the geometric and dimensional variations for each waste package due to different waste package designs, locations within the disposal system, tunnel orientations, and distance to nearest groundwater flow paths. Rather, the analytical approach is designed to reflect average or representative geometric and spatial properties. Because of this limitation, the model would not be appropriate for evaluating fine-scale system properties, such as effects of spatial variability in small-scale fracture patterns. However, the staff's extensive experience with developing and evaluating previous performance assessments supports the principle that using a representative waste package and transport pathway approach is appropriate and reasonable in a variety of applications.

- The SOAR model does not consider other biosphere pathways, such as ingestion of contaminated crops and animal products, inhalation of radionuclides on dust resuspended in air, or external exposure to radiation emitted from radionuclides on the ground surface (groundshine). It only considers ingestion of contaminated groundwater in dose calculations, which in many systems is found to be a dominant pathway.

- The SOAR model does not explicitly model geochemical processes and coupled thermal-hydrologic-mechanical-chemical processes that can affect waste package corrosion, waste form degradation, and radionuclide sorption and solubility in backfill and the geologic host media. Consideration of alternate geochemical environments can be effected by comparing model results for alternative parameter sets developed for specific geochemical environments. The initial model presented in this report includes alternative parameter sets intended to provide the users a choice of oxic or anoxic geochemical environments in fractured granite or porous media.

- The SOAR model does not consider gaseous transport of radionuclides and enhanced transport by reversible or irreversible attachment to colloids. Only aqueous phase transport of dissolved radionuclides is considered. Aqueous phase transport of radionuclides is typically considered the dominant pathway in most repository environments.

- The SOAR model does not consider nuclear criticality events (i.e., nuclear fission reactions).

- The SOAR model considers the waste package, waste form, and backfill in estimating releases from the engineered barrier portion of a geologic disposal facility. No other components of the engineered barrier system are explicitly represented.

- The SOAR model does not model complex groundwater flow and transport processes (e.g., splitting of flow paths, time-varying velocity, or varying geochemical conditions).

- Disruptive events in the SOAR model are assumed to cause damage to waste packages. Other effects, such as changes in water flow paths, are not considered.

3 OVERVIEW OF MODEL ARCHITECTURE

3.1 Model Structure

The Scoping of Options and Analyzing Risk (SOAR) model is composed of five component models that were developed using GoldSim probabilistic simulation environment software. The GoldSim simulation environment permits modular icon-based model development providing visualization of connections (influences and dependencies) between model elements. The five primary model components (Waste Form, Waste Package, Near Field, Far Field, and Biosphere) are each grouped in separate GoldSim “containers” as illustrated in Figure 3-1. A secondary model component is the Disruptive Events model component, which feeds information to the Waste Package model, such as the failure time and fraction of waste packages failed. These components were developed modularly to facilitate potential future modifications. For example, if a more detailed Waste Package model is needed, a specific container can be changed with minimal impact on the other model components. The user can take advantage of the visual display of dependencies and influences to follow the flow of information in the computations. The GoldSim user manuals (GoldSim Technology Group, LLC, 2010a,b) describe the various types of specialized GoldSim elements. Following is a brief introduction to the model components of SOAR. See the corresponding section for each model component in Chapter 4 for additional details.

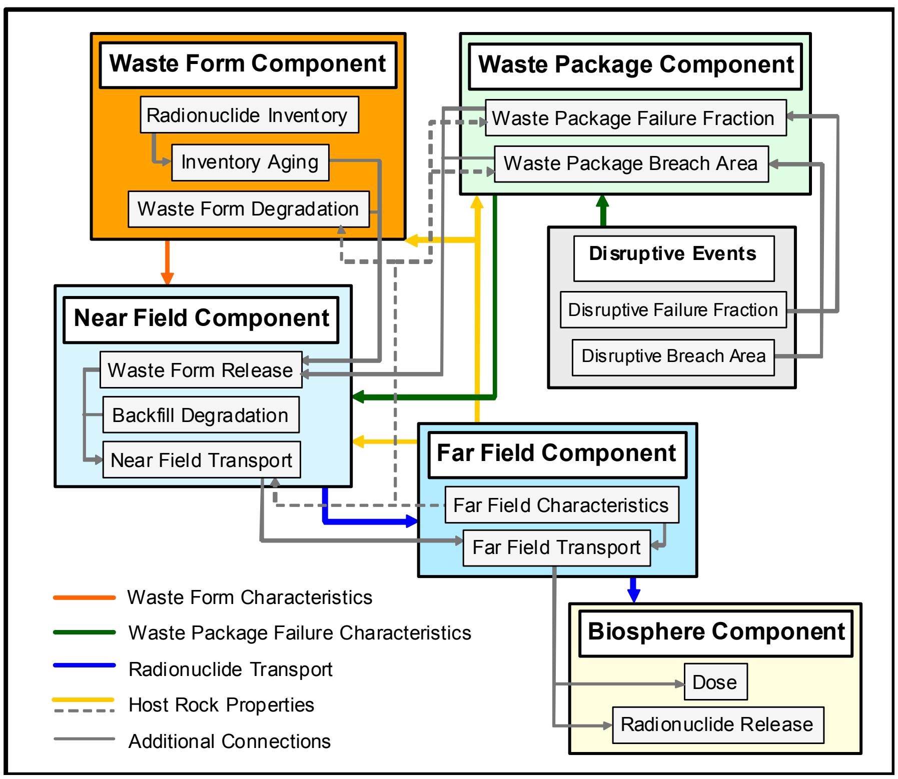

Figure 3-1. Major Model Components in the SOAR Model. Arrows Indicate Transfer of Information.

The Waste Form Component includes the radionuclide inventory and the Waste Form degradation rates. The considered waste forms in SOAR are spent nuclear fuel (SNF), high-level waste glass (HLWg) and/or high-level waste ceramic (HLWc) from reprocessed SNF, and spent mixed-oxide (sMOX) fuel. Both oxic and anoxic Waste Form degradation rates are considered.

The Waste Package Component includes the type of waste package material, abstractions for electro chemical degradation mechanisms (i.e., corrosion), and the potential opening or breached areas when failure occurs. The waste package materials considered in this initial version of the model are copper, stainless steel, carbon steel, and titanium. The main degradation process implemented is general corrosion, which computes corrosion failures for either oxic or anoxic environments, as selected by the user. An abstraction for localized corrosion is implemented for stainless steel only.

The Disruptive Events model component of SOAR can be used to consider additional waste package failure mechanisms not included in the Waste Package model component. The Disruptive Events model component specifically models three additional waste package failure abstractions.

The Near Field Component includes the characteristics of and radionuclide transport through waste package internals, any surrounding backfill, and the disturbed zone within the geologic host formation. The user can specify transport lengths of each of the three zones. In this initial version of the model, the assigned properties of the backfill zone are for a bentonite backfill (or bentonite buffer material) for which diffusion is expected to be the dominant transport mechanism. The user specifies properties of the surrounding disturbed zone to be either crystalline rock (e.g., fractured granite) or a porous rock (e.g., clay, porous media).

The Far Field Component includes the geologic media and the radionuclide transport pathways of the natural system. The geologic media were selected to encompass a range of transport pathways (e.g., matrix-dominated and fracture-dominated transport). In this initial version of the model, the input parameters for the far field are assigned to approximate transport through either fractured granite or porous sediments.

The Biosphere Component includes the radionuclide exposure and dose assessment. The dose pathway is limited to a drinking-water ingestion pathway.

3.2 Model Flexibility

Three levels of model flexibility were incorporated into SOAR and are a function of the level of modifications required to modify the model. Level one flexibility is the user-selected parameter options on the “dashboard” interface of SOAR (see Figure 3-2). Level two flexibility is modifying the default parameters. Level three flexibility is modifying the modeling elements and algorithms.

3.2.1 Level-One Flexibility: GoldSim Dashboard Variables

Level-one flexibility is incorporated into the initially parameterized version of SOAR. To exercise the level-one flexibility, SOAR has a dashboard that allows a limited set of parameter

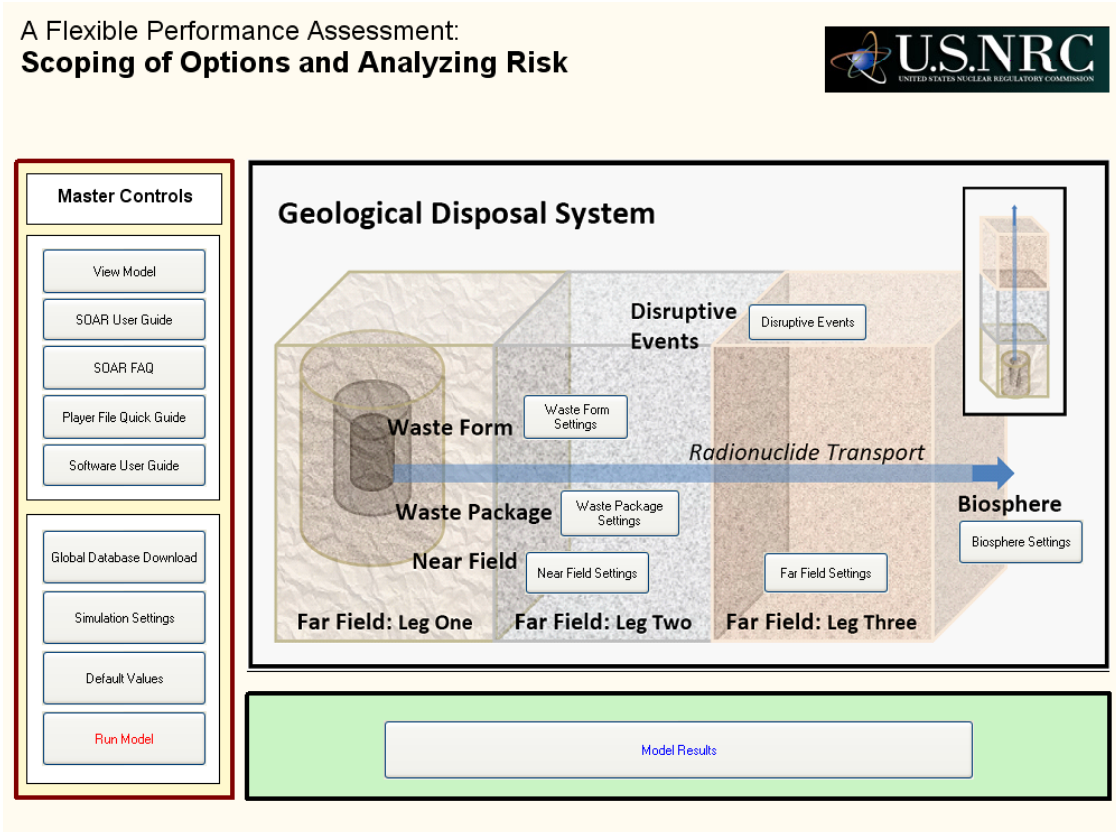

Figure 3-2. The SOAR Main Dashboard Allows Users to Exercise Level-One Model Flexibility by Selecting Predefined Parameter Sets for a Variety of Geologic Disposal System Configurations and Characteristics

combinations to be considered for simulations. Figure 3-2 shows the overall layout of the SOAR main dashboard. As shown in the figure, the dashboard provides access to level-one parameter settings for the Waste Form, Waste Package, Near Field, Far Field, Biosphere, and Disruptive Events Components. Selecting one of these options takes users to a menu of level-one settings that can be modified using the dashboard. The level-one parameters allow simulation of a wide range of potential combinations of disposal system configurations and characteristics. The dashboard also contains a set of Master Controls for running the model, viewing the model architecture, accessing this user guide and other useful information, resetting default parameters, and viewing model results. Level-one flexibility can be exercised using the GoldSim Player software, which is freely available from *www.goldsim.com*.

3.2.2 Level-Two Flexibility: Modification of Default Parameter Values

Level-two flexibility involves modifications to default model input parameter values or uncertainty distribution types. The default input parameters provided with SOAR are listed and described in Appendix A. These default values can be modified using the GoldSim Pro version.

The GoldSim Player software does not allow for model file modifications, including modifications to stochastic and data elements defining input parameters. To change model default parameter values, users need to locate the data or stochastic GoldSim element within the model, and revise the input values or distribution type as desired. For both level-one and level-two parameter modifications, there are two general classes of model parameter inputs considered in the SOAR: physical and parametric. Physical-based model inputs rely on some scientific basis or measurable quantity, such as physical dimensions of engineered barrier system (EBS) components, metal corrosion rates, diffusion coefficients, solubilities, and sorption coefficients. Parametric model inputs are intended to give flexibility to the model and account for model abstraction uncertainties. Generic enhancement factors are examples of parametric inputs. A user may obtain corrosion rates for a specific titanium alloy, and use the GoldSim Pro software to input those corrosion rates in SOAR and analyze consequences of using different waste package materials in the system. As examples of parametric-based model input modification, the user may use a scaling fraction to compute the cross section of the transition region from the backfill material to the closest fracture and explore the effect of constrained or open pathways on radionuclide releases from the EBS. The user could use the GoldSim Pro software to modify a waste form degradation-rate multiplier, for example, to explore the effect of cladding protection or the waste form degradation. Parameter modifications of this kind need an appropriate technical basis.

3.2.3 Level-Three Flexibility: Modification of Model Structure

Level-three flexibility involves modification of the model structure by adding, removing, or replacing model elements. For example, a user may develop a submodel that explicitly tracks radionuclide transport through a large fracture network. Such a model could be readily incorporated into SOAR, provided its inputs were available or implementable in SOAR. As previously stated, model structure modification requires the GoldSim Pro version.

3.3 The GoldSim Modeling Environment

SOAR was developed using the GoldSim Probabilistic Simulation Environment (GoldSim Technology Group, LLC, 2010a). With GoldSim, the model developer creates a model using a graphic simulation environment that allows users to visualize model dependencies and influences. Models developed in GoldSim can be executed in Monte Carlo mode to account for uncertainty in model inputs, such as waste package corrosion rates or radionuclide sorption coefficients. The radionuclide transport module of GoldSim provides elements to calculate radionuclide ingrowth and decay. For system requirements and additional information about GoldSim, see the GoldSim User Guide (GoldSim Technology Group, LLC, 2010a).

GoldSim allows developers to create a “dashboard” for quick user access to selected model inputs and simulation settings. Dashboard interfaces facilitate the use of GoldSim models by inexperienced users. Dashboard interfaces are also accessible with the GoldSim Player. The dashboard for SOAR, shown in Figure 3-2, allows users to easily access the level-one flexibility inputs. The SOAR dashboard includes links to documents with more detailed instructions on model use.

The SOAR model was developed using simplified models and abstractions to represent key features, events, and processes associated with geologic disposal. GoldSim has broad capabilities to incorporate internal-model documentation. Where appropriate in SOAR, additional text, figures, and hyperlinks to external documents have been provided. GoldSim allows users to control parameter inputs by providing the capability to link to an external database. SOAR uses this feature by linking to a controlled Microsoft Access database (file named FPA-SOAR.mdb). In SOAR, only physical-based parameters are controlled via the database. Flexibility parameters are directly input in dashboards or GoldSim data elements.

3.4 Quick Start Guide

The most direct way to learn to use the SOAR model is to explore a model file starting from the main dashboard. The model is provided in two formats: a GoldSim player file with a *.gsp* file name extension and a GoldSim model file with a *.gsm* file name extension. Users requiring only level-one flexibility (see Section 3.2.1) may modify dashboard parameters, run the model, and access model results of the *.gsp* file using the free GoldSim Player software. Users who require level-two and level-three flexibility (Sections 3.2.2 and 3.2.3) must work with a *.gsm* file, which requires access to GoldSim Pro to make changes to model files.

Regardless of which model format is used, opening the model will take the user to the main dashboard interface illustrated in Figure 3-2. The user may then set up the desired geologic disposal system configuration to be modeled by clicking on the buttons for waste form, waste package, near field, far field, biosphere, and disruptive events. These buttons take the user to the respective input menus illustrated in Figures 3-3 through 3-8. Moving the cursor over any of the input entries of these dashboard menus produces a pop-up text box with a description of the parameter.

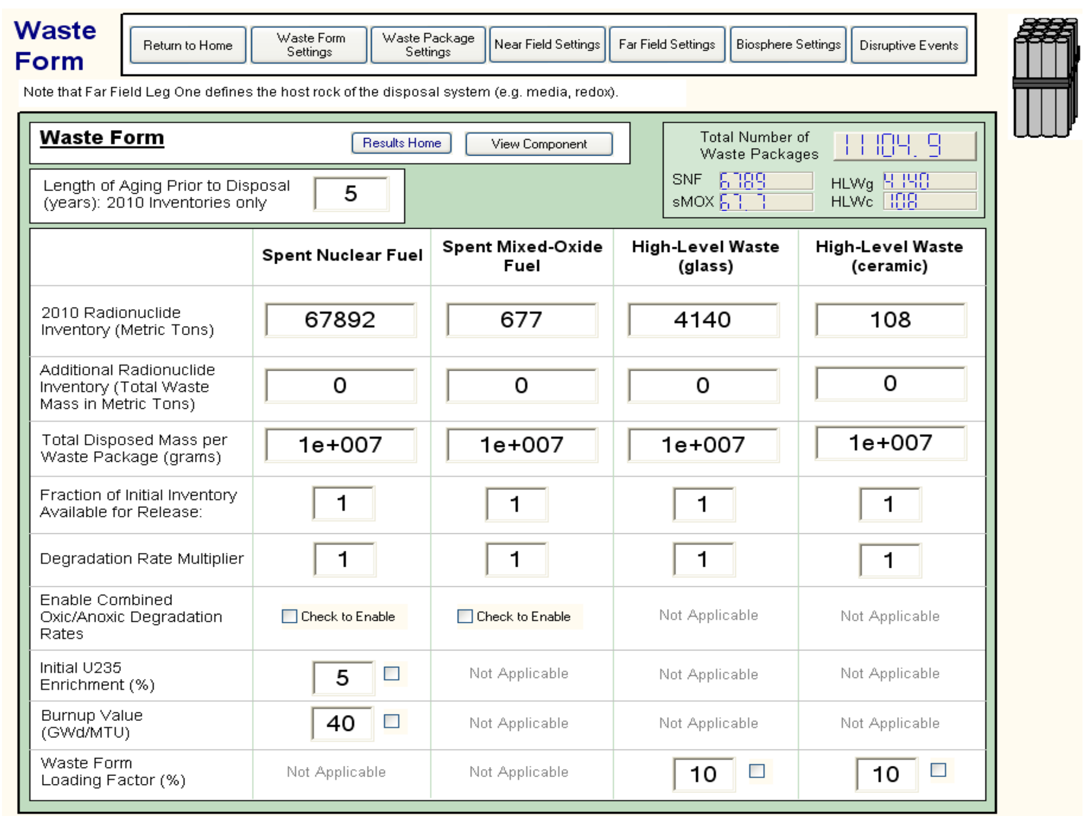

Figure 3-3. SOAR Dashboard Menu for Waste Form Model Component Configuration Inputs

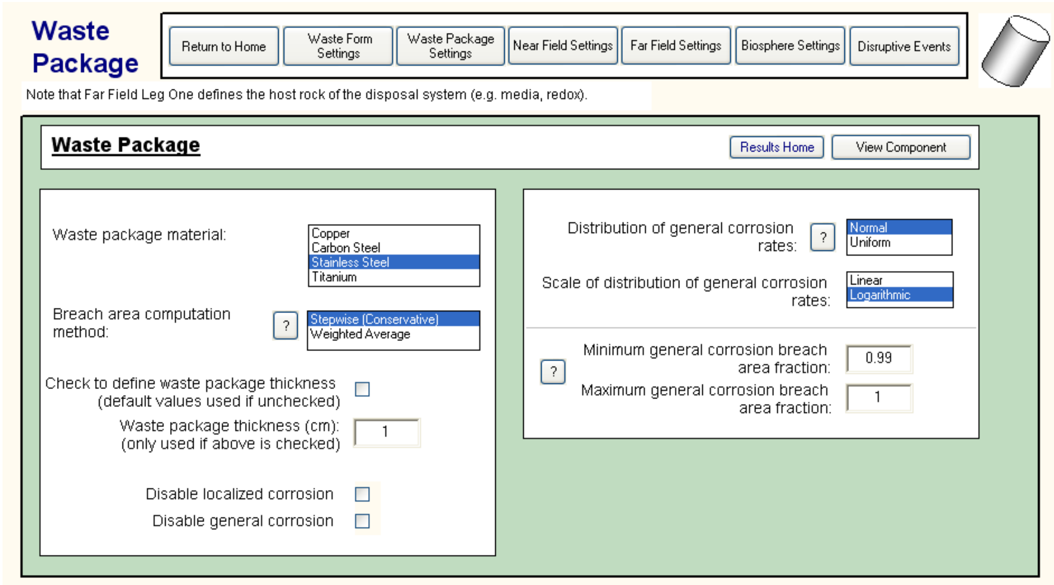

Figure 3-4. SOAR Dashboard Menu for Waste Package Model Component Configuration Inputs

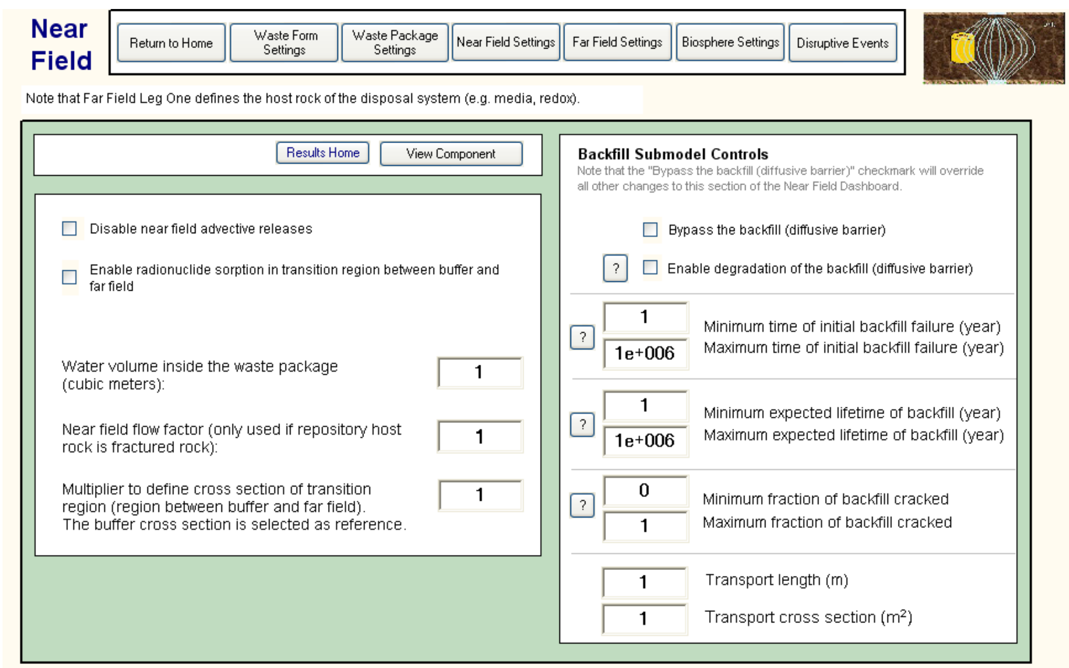

Figure 3-5. SOAR Dashboard Menu for Near Field Model Component Configuration Inputs

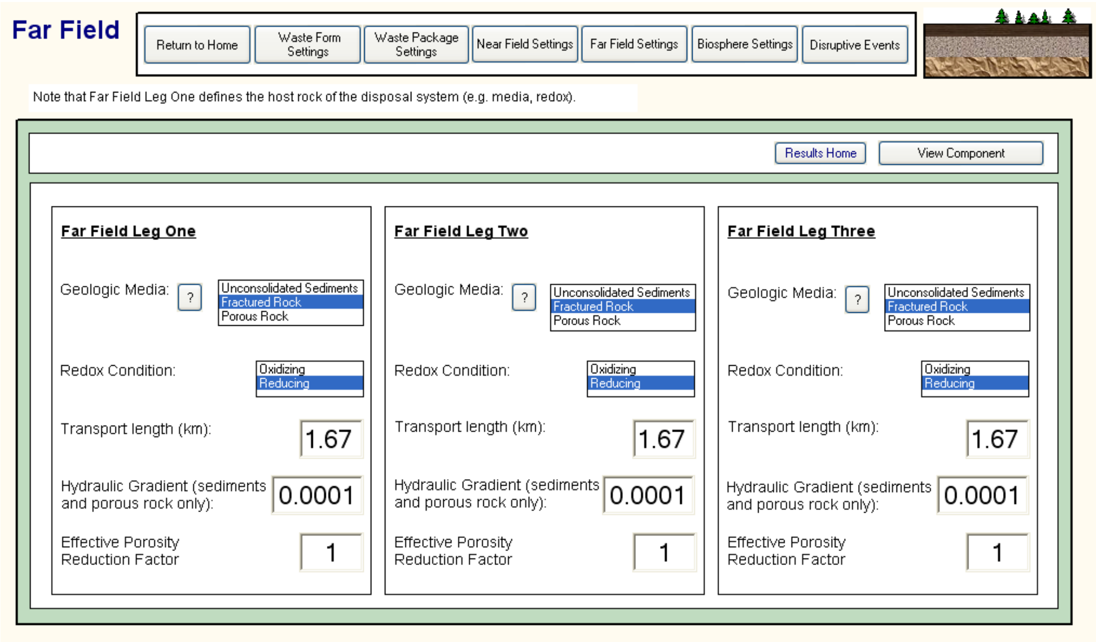

Figure 3-6. SOAR Dashboard Menu for Far Field Model Component Configuration Inputs

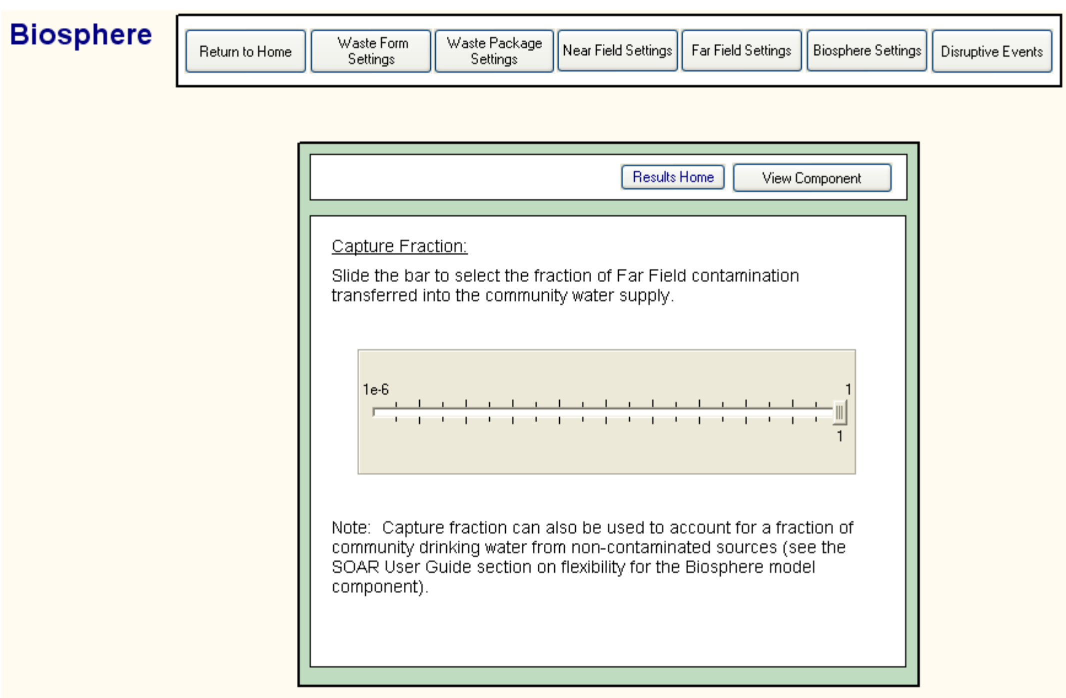

Figure 3-7. SOAR Dashboard Menu for Biosphere Model Component Configuration Inputs

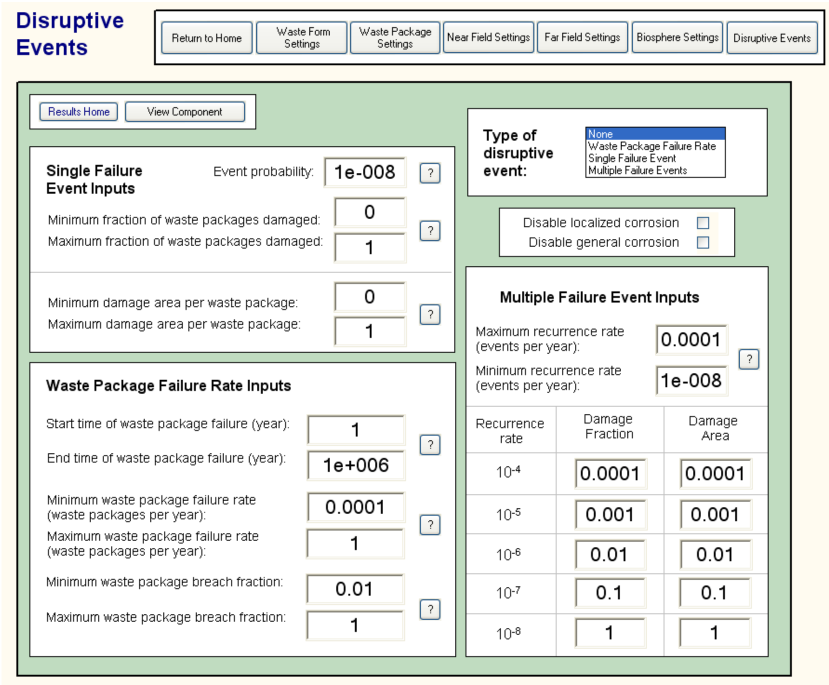

Figure 3-8. SOAR Dashboard Menu for Disruptive Events Inputs

The default values for the dashboard parameters can be restored at any time by returning to the main dashboard and clicking the “Default Values” button on the Master Controls panel (see Figure 3-2). If the model has previously been run and has stored results, the model will be in “Results Mode” and the user will not be able to make parameter changes until the model is reset. When working with the GoldSim Player version, the model can be reset by clicking the “Reset” button at the bottom of the GoldSim Run Controller, which appears as a separate popup outside the main dashboard whenever the model file is open (see Figure 3-9). There is no reset option in GoldSim Pro. Changes made using GoldSim Pro may result in different model versions. Thus, when working with *.gsm* files, users should exercise careful version control to avoid making unintended changes to default settings.

Figure 3-9. GoldSim Player Run Controller Can Be Used to Reset and Run the Model. The “Go” Button Can Be Used to Navigate the Individual Model Components.

After making desired changes in dashboard controlled entries, users can click the "Return to Home" button at the top of each menu to return to the main dashboard interface. From the main dashboard menu, the model can then be run by clicking the "Run Model" button. The model can also be run by clicking the "Run" button on the GoldSim Run Controller. If previous model results have been stored, the user will receive a warning message giving the opportunity to abort the run before overwriting previous model results. If users do not wish to overwrite a previous model, then the model with revised dashboard inputs can be saved and run in a separate folder.

After running a model, displays of model results can be viewed by clicking the "Model Results" button on the main dashboard, which will take the user to the Model Results menu shown in Figure 3-10. As can be seen in this figure, the results are grouped by the five primary model components. Figure 3-11 is an example of the dashboard results of the near field model component. In general, results are provided in graphical and tabular formats. Tabular results can be saved as separate files for post-processing or exporting to spreadsheets.

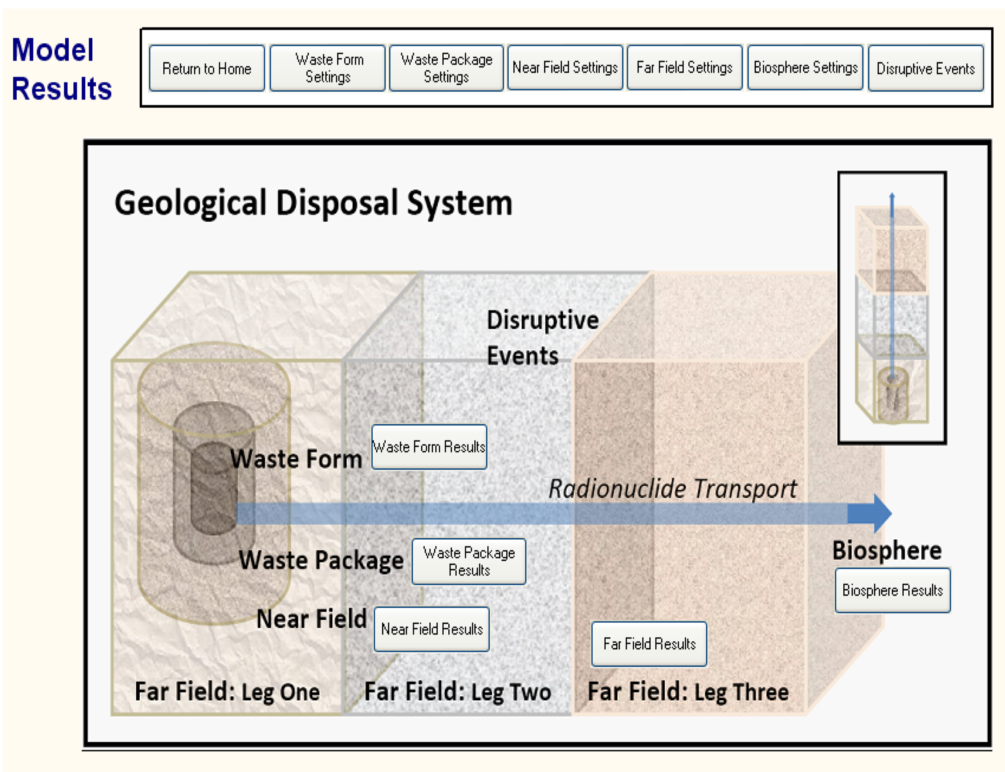

Figure 3-10. SOAR Dashboard Menu for Viewing Model Results

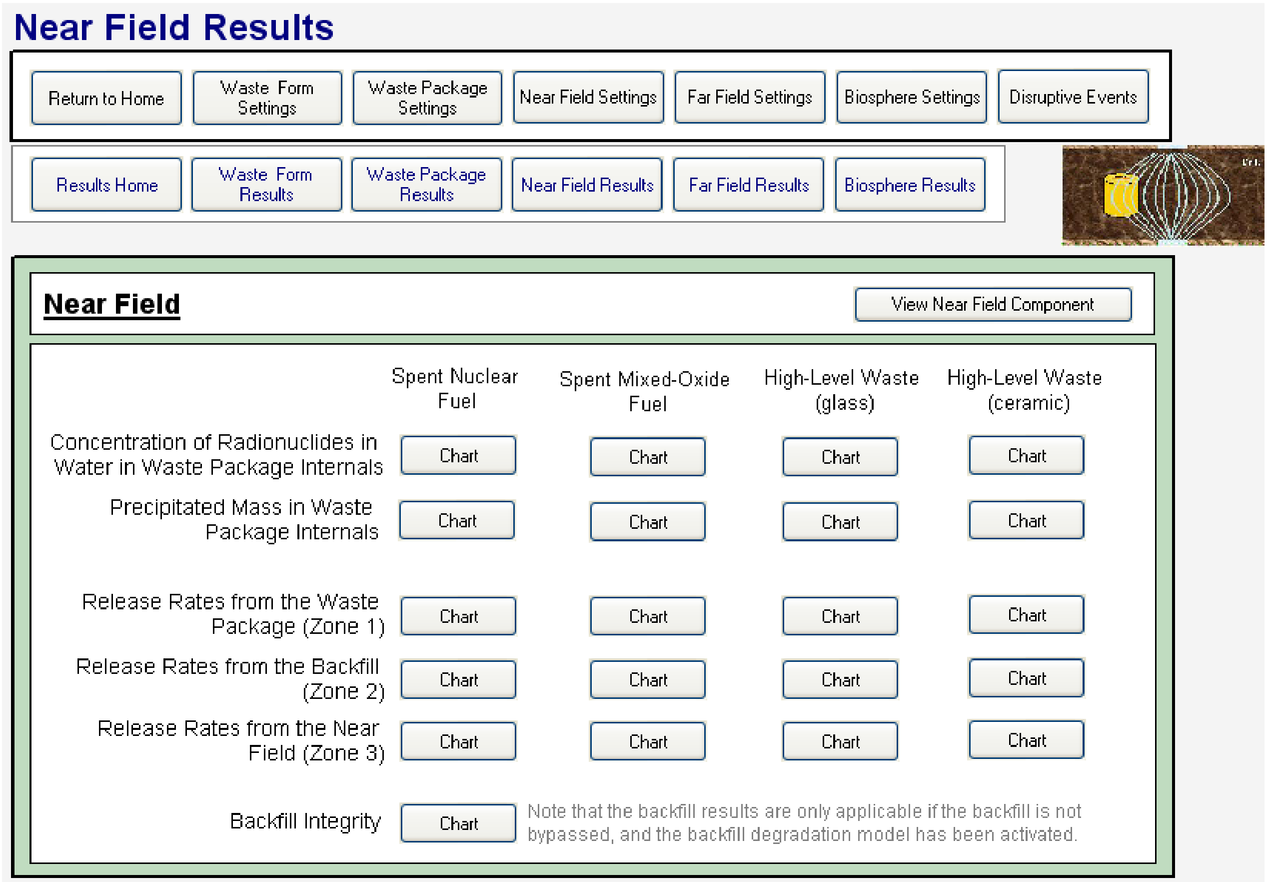

Figure 3-11. SOAR Dashboard for Near Field Model Component Results

4 MODEL COMPONENTS

4.1 Waste Form

4.1.1 Description

The Waste Form model component of Scoping of Options and Analyzing Risk (SOAR) considers the radionuclide mobilization processes from waste form dissolution to define the source term (i.e., the amount and type of radionuclides released from the waste form for radionuclide transport computations). The waste forms are emplaced inside waste packages and may be protected by cladding materials (i.e., an outer layer protecting the nuclear fuel rods to prevent radioactive fragments from escaping to the environment). The Waste Form model component specifically considers the type of solid waste form, important radionuclides, initial radionuclide inventory, and degradation of the waste form following exposure to an aqueous environment after waste package breach. The Waste Form model component is linked with the Waste Package model component and the Near Field model component. It receives waste package failure times from the Waste Package model component, which determines when water can contact the waste. The Waste Form model component outputs the mass of aqueous radionuclides mobilized at each timestep to the Near Field component.

4.1.2 Model Implementation

The model computes the amount of radionuclides dissolved from the waste form, which is then available for release as represented in the Near Field component. Sixteen radionuclide species are considered (Pu-238, 239, 240, 242; U-232, 233, 234, 235, 236, 238; Np-237; C-14; Cs-135; I-129; Tc-99; Se-79). These radionuclides were chosen to represent an appropriate variety of geochemical behaviors (e.g., mobilization) and potential waste form inventories for commercial spent nuclear fuel (SNF), spent mixed-oxide (sMOX) fuel, high-level waste glass (HLWg), and high-level waste ceramic (HLWc) waste forms, based on the performance assessment results in both oxidizing and reducing environments (Bechtel SAIC Company, LLC, 2004; Leslie, et al., 2007; Marivoet, et al., 2001). Six different radionuclide inventories are available to represent these four distinct waste forms. Each of the four waste forms (as defined in the waste form model) are individual GoldSim Source elements in the Near Field Component, one for each waste form. Each of the available waste forms has a matrix-bound inventory, which requires the waste form to degrade before the radionuclides are dissolved and released. Each matrix-bound radionuclide inventory has a characteristic dissolution rate.

In addition to the matrix-bound radionuclide inventories, two waste forms (i.e., commercial SNF and sMOX fuel) also include unbound inventories of C-14, Cs-135, I-129, Tc-99, and Se-79. These unbound inventories are instantly available for transport when the waste package breaches and are used to represent gap and grain boundary inventories. SOAR has the flexibility to add radionuclides to the inventory.

The basic equation describing the degradation rate of matrix materials is

$$\frac{dM}{dt} = -r \qquad (4\text{-}1)$$

where *M* [kg] is the mass of the matrix materials and *r* [kg/yr] is the degradation rate, considered constant in SOAR. The dissolution rates of matrix-bound radionuclides away from the waste matrix are computed by GoldSim source elements by assuming congruent dissolution with the waste form matrix. Eq. (4-1) can also be expressed as

$$\frac{dM}{dt} = -r = -g\,M_o = -R\,A\,M_o \qquad (4\text{-}2)$$

where M_o is the initial mass of the waste form matrix and g (=$R\,A$) is the initial fractional degradation rate. R [g/cm^2/yr] is the matrix dissolution rate, and A [cm^2/g] is the initial specific area of the waste form exposed to an aqueous environment. Experimental values for the dissolution rate, R, and initial specific area, A, reported in the literature for various waste forms were considered to compute initial fractional degradation rates, g, which are inputs to the Waste Form model component. From the fractional degradation rates, the waste form lifetime is computed as 1/g. The waste form lifetime is a direct input to the GoldSim source element. The dissolution rate of each radionuclide is determined by the fraction of each radionuclide in the waste form based on congruent dissolution. Complexities in the mass conservation equation arise because of the gradual waste package failure. See the Contaminant Transport Module User Guide for a more general description of the equations solved by the GoldSim source term element (GoldSim Technology Group, LLC, 2010b, Appendix E).

The four distinct waste forms selected are considered to be representative of future waste forms. Experimental data on the performance of these future waste forms are limited and are not sufficiently characterized to develop an accurate model.

4.1.3 Default Parameters

A complete list of default parameter values, distribution types, and technical bases for the Waste Form model component is provided in Appendix A, Table A–1.

For each of the four distinct default waste forms, the Waste Form model component assigns default values to the radionuclide inventory, instant release fraction of unbound inventory (i.e., fission and activation products), and fractional rate of waste form degradation.

All input data used in the Waste Form model are primarily based on published data on representative waste forms from domestic and international geologic disposal programs. To enhance traceability, data from NRC investigations are used as the initial input values when practicable, such as the instant release fraction of unbound inventory and specific surface area of the waste form (Leslie, et al., 2007; Jain, et al., 2004; NRC, 2008).

<u>Radionuclide Inventory</u>

For the four waste forms, the initial radionuclide inventories are assigned based on literature data, with an additional projection based on representative values for commercial SNF, sMOX fuel, HLWg, and HLWc. The user can modify and age the initial inventory used to account for the time that elapses before disposal system closure (e.g., HLWc with various waste loading from reprocessing). The user also has the ability to enter an additional inventory to include future waste that is generated before disposal system closure. The Waste Form model calculates the four final waste form inventories using these default and user-defined radionuclide inventories.

Instant Release Fraction of Unbound Inventory

For the unbound inventory (fission and activation products), instant release fractions for commercial SNF and sMOX fuel are determined from the values in Leslie, et al. (2007) and Jain, et al. (2004). This approach ensures that the unbound radionuclides are available for transport as soon as the waste package is breached. For higher burnup (e.g., >60 GWd/MTU) commercial SNF or sMOX fuel, the instant release fractions may increase. This approach may lead to higher estimated dose rates at earlier times. Data on unbound radionuclides for these higher burnup waste forms, however, are very limited.

Degradation of Waste Form

The Waste Form model component assumes the matrix-bound radionuclides are available for transport at the same rate as the waste form degrades. For commercial SNF, the model considers radionuclides from the matrix-bound inventory will be available for transport at the same rate as UO_2 matrix dissolution (Wilson and Gray, 1990). In an oxidizing environment, the waste form dissolution rate assumes the UO_2 matrix dissolves electrochemically as soluble species with the aid of oxidants, such as dissolved oxygen and hydrogen peroxide (Shoesmith, 2000). In a reducing environment, the waste form dissolution rate assumes the UO_2 matrix will dissolve chemically as soluble species (Sunder and Shoesmith, 1991). The Waste Form model assumes the degradation rate of sMOX fuel can be represented acceptably by commercial SNF degradation rates due to limited data on sMOX fuel degradation. This assumption accounts for uncertainties in available data on sMOX fuel degradation and similarities in sMOX fuel material properties to those of UO_2 matrix in commercial SNF. For HLWg, it is assumed that the radionuclides will be available for transport at the degradation rate of the HLWg matrix. This rate assumes the HLWg matrix will dissolve chemically, where the process is controlled by the concentration of dissolved silica compound in both oxidizing and reducing environments (Bechtel SAIC Company, LLC, 2004). HLWc has been studied only in laboratories. There is no prototype HLWc. A variety of HLWc waste forms have been considered (e.g., SYNROC, titanates, zirconolites). The HLWc typically have lower degradation rates than HLWg (Wang, 2009). From the limited laboratory data (Reeve, et al., 1989; Vance, et al, 1997; Wang, 2009), a decreasing factor of 0.01 is chosen for HLWg degradation.

To determine the fractional degradation rate for each specific waste form, upper and lower bounds for waste form dissolution rate were considered for both oxic and anoxic conditions and for various pH conditions, based on representative values in the literature (e.g., NRC, 2008; Van Iseghem, 2007; Ferry, et al., 2005; Bechtel SAIC Company, LLC, 2004). These bounding values for the dissolution rate were then multiplied by the specific surface area of the waste form, accounting for the waste form density and surface roughness factors (NRC, 2008). In computing fractional degradation rate inputs to the Waste Form model component, specific surface areas were considered, using a waste form size (diameter or edge size) of 0.1 cm [0.04 in] for commercial SNF and sMOX fuel (NRC, 2008) and 10 cm [4 in] for HLWg (Bechtel SAIC Company, LLC, 2004). The densities are 10.6 g/cm^3 [0.38 lb/in^3] for commercial SNF and sMOX fuel (NRC, 2008) and 2.7 g/cm^3 [0.1 lb/in^3] for HLWg (Ahn, 2003). The resulting fractional degradation rates were used to define upper and lower limits for log-uniform distributions, which are sampled once in each realization to account for uncertainty in fractional degradation rates for each waste form.

In the Waste Form model component, a constant degradation rate is assumed [see Eq. (4-1)]. This assumption simplifies the calculation procedure without underestimation of radionuclide release from the waste form. The dissolution rate and specific surface area, however, could vary over time for different waste forms, environmental conditions, and geometrical considerations. The time-dependent data on waste form degradation rates for the range of potential environmental conditions and future waste form types is limited and should be studied further in the future to address uncertainties. In connection to the waste package failure over time, the use of one representative waste package material in the Waste Package model component assumes that when the waste packages breach, they simultaneously expose the waste forms to an aqueous environment. However, waste package designs (e.g., wall thickness, fabrication methods, welding process) could be different depending upon the waste form contained. These differences could lead to different failure times of the waste packages, resulting in different aggregated radionuclide releases.

4.1.4 Flexibility

In addition to the default parameterization, the Waste Form model has several significant flexibilities. For example, the user can modify the default parameter values for the waste form inventories and fractional degradation rates of commercial SNF, sMOX fuel, HLWg, and HLWc To account for aging of the initial 2010 radionuclide inventories prior to disposal system closure, the user has the flexibility to specify the length of aging. The user can include future waste by specifying additional radionuclide mass for each of the four waste forms. For the commercial SNF, the additional radionuclide inventory is generated from a look-up table (Sippel, et al., 2011) using specified values for initial fuel U-235 enrichment and fuel burnup. The user has the flexibility to input values for the fuel enrichment and burnup or to select that either parameter be sampled from a representative distribution. For HLWc, the additional radionuclide inventory added uses the radionuclide composition from the default HLWg waste form. This is done to more closely approximate potential waste stream compositions from reprocessing. The user also has the flexibility to change the total disposed mass per waste package for each of the four waste forms. These parameters are used in calculating the number of waste packages and affect the calculation of the waste package failure distribution. The user can modify these values to study the effects of waste package mass loading and varied number of waste packages on system performance. To represent the case of potentially higher loading concentrations of HLWg and HLWc, the user can modify the mass of radionuclides for these waste forms through use of inventory loading factor parameters. The user can modify the releasable fraction of the initial radionuclide inventory for each waste form, which is the fraction of the waste form mass that is made available for mobilization. This fraction may decrease the inventory available for transport (e.g., to simulate the effects of potential cladding protection for radionuclides mobilized or change of local redox condition). The user can modify the fractional rate of waste form degradation using a multiplier that is applied to the bound inventory degradation rate for each waste form. This parameter can be used to approximate effects that may either increase or decrease the bound inventory degradation rates (e.g., the user could assume different waste form fragment sizes and modify the degradation rate accordingly). A combined oxic/anoxic degradation rate can also be used to approximate the effects of water radiolysis (dissociation of water molecules by alpha or gamma radiation to produce highly reactive radicals, such as oxygen and hydrogen peroxide) on waste form degradation in an anoxic environment.

The Source Term menu of the user interface dashboard (see Section 3.4) allows users additional flexibility to evaluate alternative model concepts without the need to revise the input parameter distributions.

Specifically, the dashboard provides users with the options to

- Specify the length of aging prior to disposal for the initial 2010 radionuclide inventory
- Specify additional radionuclide inventory for commercial SNF, sMOX fuel, HLWg, and HLWc
- Specify the total disposed mass per waste package for commercial SNF, sMOX fuel, HLWg, and HLWc
- Specify the values of degradation-rate multipliers for commercial SNF, sMOX fuel, HLWg, and HLWc
- Specify the releasable fractions of commercial SNF, sMOX fuel, HLWg, and HLWc
- Specify the inventory loading factors of HLWg and HLWc

4.2 Waste Package

4.2.1 Description

The Waste Package model component of SOAR specifically models waste package chemical degradation (i.e., corrosion) processes that may lead to waste package failure. Additional waste package failures caused by disruptive events are modeled independently in the Disruptive Events model component as described in Section 4.6. The Waste Package model component calculates waste package failure times and the extent of damage on the waste package surface for geologic disposal systems located in either oxidizing or reducing host media, where the redox condition of the geologic media is defined by the first leg of the Far Field component. The Waste Package model component is integrated with the Disruptive Events, Waste Form, and Near Field model components. The Waste Package model component receives the fraction of waste packages failed by disruptive events and the disruptive event breached area fraction from Disruptive Events model component and combines them with those analogous outputs from this Waste Package model component to calculate a combined breached area. The Waste Package model component provides the waste package failure times to the Waste Form model component to initiate computations of waste form degradation for each failed waste package and the total breached areas to the Near Field model component for radionuclide transport calculations.

4.2.2 Model Implementation

The Waste Package model component calculates waste package failure times and breach area fractions for some materials due to corrosion in aqueous environments, representing some potential conditions for a geological disposal system. The calculation considers the following attributes of the Waste Package model component.

<u>Waste Package Specifications</u>

It is assumed the disposal system will include waste packages made of a single metallic material. The Waste Package model component considers general corrosion and localized corrosion (where applicable) for either stainless steel, carbon steel, titanium, or copper. These materials were selected to represent those susceptible to corrosion and those that are corrosion resistant. Depending on the material type and chemical environment (oxidizing or reducing) the user selects on the dashboard interface, the model will choose the appropriate set of parameter values to use in calculating waste package failure times and breach areas.

<u>Failure Mechanisms (General Corrosion and Localized Corrosion)</u>

The Waste Package model component models two waste package failure mechanisms representing general corrosion and localized corrosion. General corrosion is modeled to represent progressive failures of waste packages distributed over time. Conversely, localized corrosion is modeled to breach a fraction of the surface of the waste packages at discrete times. Other degradation processes (e.g., stress corrosion cracking, microbial influenced corrosion, hydrogen embrittlement, creep, and susceptibility to corrosion as a function of metal and container fabrication processes) are not explicitly considered in the model. The following paragraphs describe the calculation process for general and localized corrosion.

General corrosion is assumed to be a gradual material thinning process proceeding in a relatively slow and uniform manner compared to localized corrosion. The waste package failure time is calculated as the time at which the corrosion front penetrates the material thickness, using the equation

$$t_{gc} = \frac{L}{R_{gc}} \qquad (4\text{-}3)$$

where t_{gc} is the waste package failure time by general corrosion, L is the thickness of waste package material, and R_{gc} is the general corrosion rate in units of length/time.

The distribution of general corrosion rates for the respective waste package materials is an input to the general corrosion model in the Waste Package model component. In a realization, each waste package is considered to exhibit a single corrosion rate. The complete distribution of corrosion rates is covered by the multiple waste packages. Thus, waste packages are computed to fail at different times within a realization, depending on their corrosion rate. In the model, general corrosion rates are limited to follow either normal or uniform distributions, or their logarithmic variants, with user-defined lower and upper bounds. In the case of normal or lognormal distributions, the lower and upper bounds correspond to the 0.1 and 99.9 percentiles of the failure time distribution. In the case of uniform or log-uniform distributions, the low and high bounds are the minimum and maximum failure rates. The effect of surface roughness potentially developed in the long term may need to be considered in the future in determining the distribution type for general corrosion times.

Localized corrosion is modeled as a relatively fast degradation process compared to general corrosion leading to waste package failure in a stepwise manner. No explicit models for initiation and propagation of localized corrosion are implemented. Instead, failure times are directly sampled from input distributions. Localized corrosion is assumed to cause waste package failure at different, discrete times depending on whether the geologic disposal system is located in reducing or oxidizing host media.

For a disposal system located in reducing host media, an initial transient oxidizing period (referred to as Period I) is considered before a stable reducing condition is established (referred to as Period II). The initial transient oxidizing period is assumed to be much shorter than the stable reducing period because the initial oxygen in the disposal system in a reducing host media is reported to be consumed primarily by the corrosion process in tens to hundreds of years. For this type of disposal system, a two-step function defining the fraction of waste packages affected by localized corrosion (f_{lc}) as a function of time is constructed for each realization, as shown in Figure 4-1. Two distributions to define the waste package failure time by localized corrosion (t_{lc}) are provided as inputs to the Waste Package model component, one for Period I and the other for Period II. Other inputs to the Waste Package model component are the fractions of waste packages affected by localized corrosion during Periods I and II. During Period I, the affected fraction is sampled from a distribution for f_{lc}, which was selected based on the probability that a waste package will exhibit localized corrosion under the transient oxidizing conditions.

During Period II, it is assumed that waste packages that did not fail in Period I could still exhibit localized corrosion. The fraction of waste packages failed during Period II is sampled from a distribution based on the probability for a waste package to exhibit localized corrosion under reducing conditions. This stepwise failure model allows the user to consider localized corrosion failures at two discrete times. The total number of waste packages that fail by localized corrosion is the sum of the number of waste packages failed during both Periods I and II, as shown in Figure 4-1.

In the case of a disposal system in oxidizing host media, only one failure time distribution is provided as an input to the Waste Package model component, along with the corresponding distribution for the fraction of waste packages affected by localized corrosion. With these inputs, a single-step function defining the fraction of waste packages failed by localized corrosion as a function of time is constructed for each realization, as shown in Figure 4-1. The fraction of waste packages failed by localized corrosion is sampled from a distribution based on the probability for a waste package to exhibit localized corrosion under oxidizing conditions.

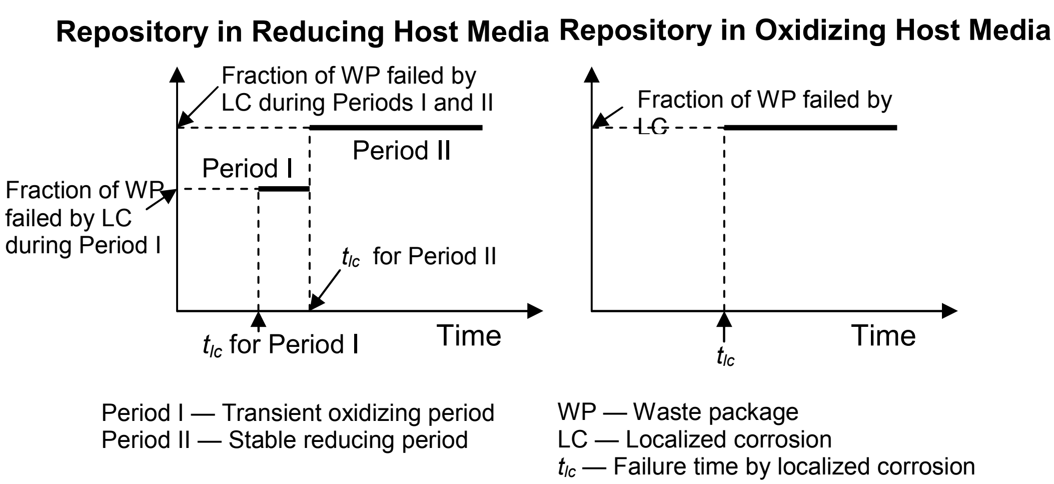

Figure 4-1. Step Functions Used to Model Localized Corrosion Per Realization

Waste Package Breached Area

An output of the Waste Package model component is the combined waste package breached area from corrosion processes and disruptive events, described in Section 4.6, as a function of time. This breached area is provided as input to the Near Field component. Diffusive radionuclide releases into the region surrounding the waste packages are proportional to this breached area (see Section 4.3.2 for a discussion on advective radionuclide releases). SOAR considers three distinct breached area fractions: one for localized corrosion, one for general corrosion, and one for disruptive events. For waste package radionuclide release computations, however, a combined breached area per failed waste package is computed at each timestep as a function of each distinct breached area and the number of waste packages failed.

Two different approaches in SOAR were implemented to compute the breached area per failed waste package as a function of time, and the user can select the approach to use. The first is a stepwise approach. In this approach, to compute the breached area by corrosion at a timestep, whether the waste packages failed by general corrosion or localized corrosion is considered. If only waste packages failed by localized corrosion or general corrosion are present at that timestep, the corresponding sampled value for the breached area fraction by localized corrosion or general corrosion is used to compute the breached area. If waste packages failed by both localized corrosion and general corrosion are present at a timestep, the breached area fraction is computed as the sum of the fractions associated with localized corrosion and general corrosion. This is equivalent to assuming that all failed waste packages experience both localized corrosion and general corrosion. Therefore, this approach overestimates the breached area per failed waste package as only a few (not all) waste packages would experience both corrosion processes. In this stepwise approach, if only waste packages failed by disruptive events are present at a timestep, the combined breached area is determined from the timestamp associated with the disruptive events (see Section 4.6.2). If waste packages failed by corrosion are also present at that timestep, the combined breached area per failed waste package is defined as the maximum of two quantities: (i) the area breached by corrosion only and (ii) the area breached solely by disruptive events. For general corrosion leading to gradual failure, the waste packages failed are assumed to be present in the system at timesteps greater than the time required for the waste package with the highest general corrosion rate (or the 99.9 percentile corrosion rate if corrosion rates follow a normal distribution) to fail.

In the second approach, the breached area per failed waste package, $WP_{breached\ area}$, is computed as a weighted average:

$$WP_{breached\,area} = \left(\frac{f_{gc}}{f_{failed\,WP}} f_{gc\ breached\ area} + \frac{f_{lc}}{f_{failed\,WP}} f_{lc\ breached\ area} + \frac{f_{de}}{f_{failed\,WP}} f_{de\,breached\,area}\right) A \tag{4-4}$$

where f_{gc} is the fraction of waste packages failed by general corrosion, $f_{failed\ WP}$ is the fraction of waste packages failed, $f_{gc\ breached\ area}$ is the general corrosion breached area fraction, f_{lc} is the fraction of waste packages failed by localized corrosion, $f_{lc\ breached\ area}$ is the localized corrosion breached area fraction, f_{de} is the fraction of waste packages failed by disruptive events from Section 4.6.2, $f_{de\ breached\ area}$ is the disruptive event breached area fraction from Section 4.6.2, and A is the total area of a waste package. In this equation, if few waste packages are failed due to general corrosion and the majority of the waste packages are failed by localized corrosion, the breached area per failed waste package is closer to the breached area associated with localized corrosion. As more waste packages fail due to general corrosion, the breached area per failed waste package, $WP_{breached\ area}$, approaches the breached area associated with general corrosion.

As stated previously, localized corrosion is modeled to be a faster degradation process than general corrosion. If localized corrosion failure occurs, it usually occurs prior to general corrosion failure. As such, the stepwise approach calculates a breached area that is greater than calculated with the weighted average approach.

4.2.3 Default Parameters

A list of default parameter values, distribution types, and technical bases for the Waste Package model component is provided in Appendix A, Table A–2. The default parameters in the Waste Package model component assign values to assess consequences of general corrosion and localized corrosion of the waste package. General corrosion affects all waste package materials in both oxidizing and reducing conditions, while localized corrosion only affects particular materials (stainless steel in the current SOAR version).

For the general corrosion model, the key input parameters are the general corrosion rates for each waste package material for geologic disposal systems in oxidizing or reducing media [R_{gc} in Eq. (4-3)] represented as probability distributions to reflect uncertainties in the disposal system environmental conditions. Environmental conditions affecting general corrosion (e.g., temperature, solution pH, and solution chemical composition) are not explicit inputs to calculate general corrosion rates. Nevertheless, their influence is implicitly accounted for by the specified ranges of the corrosion rate distributions (i.e., the lower and upper bounds for the distributions are obtained from literature data representing benign and aggressive environmental conditions). Other general corrosion inputs include the thickness of each waste package material [L in Eq. (4-3)] and general corrosion breached area fraction [$f_{gc\ breached\ area}$ in Eq. (4-4)] sampled from the user-defined breached area fraction range for general corrosion on the dashboard interface.

For the localized corrosion model, a key parameter is the probability of waste package failure by localized corrosion, which differs for the four materials considered in the SOAR default parameter set. For example, the titanium waste package material is assumed to be alloyed with noble metals (e.g., palladium or ruthenium), which effectively prevents localized corrosion of this material (e.g., Revie, 2000). Accordingly, the localized corrosion probability parameter is set to zero for this material. For copper and carbon steel, localized corrosion in the form of pitting corrosion is considered possible. The localized corrosion probability parameter, however, is also set to zero because localized corrosion of these materials is not explicitly modeled with the localized corrosion model. Instead, localized corrosion is indirectly modeled by enhancing the general corrosion rates provided as input, because pitting corrosion of these materials is more widespread (e.g., Revie, 2000). The extent of the enhancement is not an explicit input to the general corrosion model. As previously stated, the effect of pitting is implicitly accounted for in the selection of distributions of general corrosion rates. Other inputs to the localized corrosion model include localized corrosion failure time (t_{lc} in Figure 4-1) and localized corrosion breached area fraction [$f_{lc\ breached\ area}$ in Eq. (4-4)].

The parameter values used in the waste package component were primarily obtained by literature review of waste container design and corrosion testing results from domestic and international geologic disposal programs. Independent analyses and engineering judgment were also used where data were lacking, such as to establish the probability and breach area fraction for localized corrosion of stainless steel.

4.2.4 Flexibility

In addition to the default parameterization, the Waste Package model component has several flexibilities to consider alternative geologic disposal system configurations. Where appropriate technical data are available, the user can modify the general corrosion rates to assess performance of other waste package materials (see discussion of level-two flexibility in Section 3.2). These corrosion rates can be modified to constrain uncertainty where environmental conditions in the disposal system are better characterized or to analyze different environmental regimes (e.g., increasing the rates due to higher temperatures). The user can modify the distributed and stepwise failure to approximate additional failure mechanisms beyond general and localized corrosion. Given that any waste package failure mechanism can be characterized by two quantities—the failure time and the extent of damage to the waste package surface—the user can adjust the default input parameters to evaluate consequences of other failure mechanisms. For example, consequences of stress corrosion cracking could be evaluated, provided technical data were available to define the extent of waste package surface damage and other input parameters selected to cause failure in expected time frames. Similarly, the user can modify the stepwise failure time, probability, and breach area fraction to approximate discrete events, such as early failure, human intrusion, or other disruptive events. Note that because SOAR is an abstracted scoping tool with limited consideration of coupling among processes leading to waste package failure and radionuclide release to the environment, the results should be carefully interpreted.

The Waste Package menu of the user interface dashboard (see Section 3.4) allows users additional flexibility to evaluate alternative model concepts without the need to revise the input parameter distributions. Specifically, the dashboard provides users with the options to

- Specify the waste package material
- Define a waste package thickness, thus overruling default thickness values for each specific material (see Appendix A, Table A–2 for default values)
- Disable general corrosion or localized corrosion degradation modes
- Specify distribution type (normal or uniform) and scale (linear or logarithmic) of general corrosion rates
- Define breached area fraction range for general corrosion
- Specify breached area computation approach [stepwise from Figure 4-1, or weighted average from Eq. (4-4)]
- Select reducing or oxidizing geochemical environment (selection made under the Far Field model component menu)

4.3 Near-Field Environment

4.3.1 Description

The Near Field component of SOAR considers transport of radionuclides from within the waste package, through the disturbed zone outside the waste package, and into the undisturbed natural system. The Near Field component of SOAR specifically considers dissolved radionuclide transport through any engineered buffer and/or backfill materials accounting for the effects of advection, dispersion, diffusion, sorption, and mineral precipitation and dissolution. The Near Field model component receives dissolved radionuclide releases from the Waste Form model component, receives breach area from the Waste Package model component, and provides dissolved radionuclide releases to the Far Field model component.

4.3.2 Model Implementation

The Near Field model component uses a one-dimensional diffusive and advective transport approach with sorption and mineral precipitation and dissolution. Conceptually, the model considers dissolved radionuclide transport from the near field to the far field through three distinct transport zones: (i) from the waste package internals through the breach area, (ii) from the surface of the waste package through any engineered buffer or backfill material, and (iii) a transition region from the buffer or backfill material to a far-field groundwater transport pathway. The SOAR model includes four independent subsystems, one for each waste form that tracks inventories: (i) waste form dissolution, (ii) solubility and precipitation, (iii) contaminant transport through the buffer or backfill material, and (iv) contaminant transport through the transition region. Each of these four subsystems tracks a number of waste packages, as defined in the dashboard for the Waste Form model component (see Section 4.1). The same fraction of waste packages failed as a function of time computed by the Waste Package and Disruptive Event model components is used in the four subsystems. Likewise, the same breach area fraction as a function of time computed by the Waste Package and Disruptive Event model components is used in the four subsystems. Zones 1, 2, and 3 common to the four subsystems are discussed next.

In zone 1, two processes are considered. First, dissolved concentrations of radionuclides released from the waste form are computed. For radioactive species with relatively low solubility (e.g., uranium and plutonium), solid phases may precipitate from solution and constrain the dissolved concentration to the solubility limit. Concentrations of highly soluble radionuclides (e.g., cesium and iodine) are unlikely to reach their solubility limits, and concentrations are controlled only by the waste form degradation rate relative to the release rate from the waste package. The second process considered in zone 1 is radionuclide releases into zone 2. Mass balance equations governing advection, dispersion/diffusion, and radionuclide decay are solved using the GoldSim cell network implementation (GoldSim Technology Group, LLC, 2010b).

The radionuclide release rates are computed based on flow rates (advective transport), concentration difference (diffusive transport), and the cross-sectional area of breaches in the degraded waste package using the GoldSim cell network representation of the mass balance equation

$$f_{bs} = c_s v + D_s \left(c_s - c_b \right) \qquad (4\text{-}5)$$

where f_{bs} is the release rate (g/yr), v is the flow velocity out of the waste package (m^3/yr), c_s is the radionuclide concentration in water inside the waste package (g/m^3), c_b is the radionuclide concentration in water outside the waste package (g/m^3), and D_s is the diffusive conductance (m^3/yr). The diffusive conductance term in Eq.(4-5) is calculated as follows

$$D_s = \frac{WP_{breached\ area}}{\dfrac{L_i}{n_i D_{is} \tau_i} + \dfrac{L_b}{n_b D_{bs} \tau_b}} \tag{4-6}$$

where $WP_{breached\ area}$ is the waste package breached area (m^2); L_i and L_b are the diffusive lengths of the mixing cell immediately inside and outside the waste package, respectively (m); n_i and n_b are the porosity of the mixing cells *i* and *b*, respectively; D_{is} and D_{bs} are the diffusivity of species *s* in the water of mixing cells *i* and *b*, respectively (m^2/yr); and τ_i and τ_b are the tortuosity of the porous medium within mixing cells *i* and *b*, respectively. The term $WP_{breached\ area}$ is the combined breached area that includes contributions from general corrosion, localized corrosion, and disruptive events. The approach to compute the combined breached area is described in Section 4.2, Eq. (4-4).

Radionuclide release rates are constrained by solubility limits. The solubility constraints on concentration are enforced within the GoldSim mixing cell representing the waste package internals. This mixing cell tracks the mass of radionuclides released from the waste form as well as the mass transferred to zone 2. The GoldSim mixing cell keeps track of the precipitated mass, which can be dissolved back when the concentration falls below the solubility limit. The net effect of the solubility limit is to increase the residence time of radionuclides in the mixing cell representing the waste package internals.

Equation (4-5) accounts for both advective and diffusive release mechanisms. For calculation of advective release, it is assumed that water can flow through the waste package (i.e., v>0) only if the diffusive barrier capability of the backfill region (zone 2) is degraded or absent. Hence, there is no advective transport in zone 1 as long as zone 2 is intact (see zone 2 discussion in next paragraph). Diffusive release occurs regardless of the state of zone 2. Therefore, in simulations where backfill degradation is not enabled, diffusive transport is the only mechanism for release away from the waste package.

In zone 2, dissolved radionuclides are transported through the engineered buffer or backfill material. For sorbing radionuclides, transport is delayed by sorption into the buffer material. Solubility constraints are also applied to the radionuclide concentrations in zone 2. Three options for the treatment of the diffusive barrier capability of the backfill are available through settings in the dashboard: always intact, degraded over time, or backfill bypass. For an always intact zone (default case), radionuclide transport occurs only by diffusion in the direction of the concentration gradient. If degradation over time is selected (by checking the “Enable degradation of the backfill” option in the dashboard), it is assumed that the number of waste packages with degraded diffusive barriers increases over a defined time period (i.e., the user specifies an initial failure time and an expected lifetime) and that each degraded diffusive barrier exhibits a maximum cracked area (also user defined) at the time of failure. Degraded diffusive barrier units allow for water flow through the cracked region and for advective radionuclide transport. Advective releases are proportional to the fraction of degraded diffusive barrier units. In the backfill bypass option, flowing water is assumed to contact the waste form at a rate determined by flow parameters for the first leg of the far-field component, and zone 2 is absent (i.e., radionuclides are transported directly into zone 3).

In zone 3, or the transition region, dissolved radionuclides are transported from the diffusive barrier to the closest fracture (for a disposal system in fractured host rock) or to the rock matrix (for a disposal system in porous rock) via diffusion and advection. Transport through this region is handled differently depending on whether the host rock is fractured rock or porous medium. If the host rock is a porous medium, the diffusive transport distance for this zone is set to an extremely low value (10^{-8} m for current basecase) and releases from zone 2 effectively go directly to the far-field (i.e., first leg of the far-field). For a disposal system located in porous rock, it is implicitly assumed that water approaching the engineered buffer has a low concentration, represented by a zero concentration boundary at the formation next to the diffusive barrier. In other words, it is assumed that fresh water outside the diffusive barrier transports radionuclides away at a rate much faster than they are released, which results in a steeper concentration gradient in zone 2 Radionuclide release into the host rock is due to both diffusion and advection. As in the fractured rock case, flow velocities for a porous medium in zone 3 are consistent with flow velocities in the transport computations for leg 1 of the far-field (see Section 4.4 for description of the Far Field model component). The model contains flexibility to enable or disable sorption in the host rock within this transition region.

For a fractured host rock, the effective transport distance to the far field flow pathway is proportional to the fracture separation, with a proportionality constant that is randomly sampled to account for the fact that waste packages are randomly located with respect to the nearest fracture. Flow velocities through the fracture are consistent with flow velocities in the first leg of the far-field. That is, flow velocities through the transition region are considered proportional to the far-field fracture-flow velocity, with a user-specified proportionality constant. This proportionality constant allows flexibility to account for factors that can cause the flow rate in the near-field transition zone to differ from the main far-field transport pathway. For example, if the transition region is relatively unfractured and minimally disturbed during construction, advective flow rates would be low. In this case, a proportionality constant might be estimated from the ratio of far-field fracture permeability to the near-field matrix permeability. For the diffusive component of transport in zone 3, the far-field interface at the end of the transition region is modeled as a zero-concentration boundary. Therefore, if the fracture spacing is wide, the effective transport distance is longer, resulting in a lower concentration gradient, which in turn reduces the rate of diffusive radionuclide release into the far-field. Assumptions include the following:

- Sorption of dissolved radionuclides onto solid material occurs instantaneously and is described by an equilibrium partition coefficient (k_d) for a specified environment (i.e., it is an instantaneous equilibrium linear sorption model).

- Precipitation/dissolution reactions are reversible. A single mineral phase controls the solubility for each element for a specified set of geochemical conditions. Radioisotopes of a single element share the same solubility constraint. For example, the concentration of dissolved uranium in water leaving the waste package is computed by adding all the concentrations of the uranium isotopes present at that time. If the total concentration exceeds the solubility limit, then uranium minerals form that include proportional amounts of the uranium isotopes.

- The pH, ionic strength, pCO_2, and oxidation state do not vary spatially or temporally in the near-field. For a specified geochemical environment, a range of these parameter values can be considered using a distribution of solubility constants and partition coefficients.

4.3.3 Default Parameters

A complete list of default parameter values, distribution types, and technical bases for the Near Field model component is provided in Appendix A, Table A–3.

The diffusion coefficient, dispersion coefficient, solubility limit, and partition coefficient parameter values or ranges of values used for various engineered barrier materials in the Near Field model component were primarily obtained by literature review of engineered barrier designs, laboratory testing, and geochemical modeling results from domestic and international geologic disposal programs. Based on the user's selection of redox conditions for a simulation, the model will select representative input data distributions for radionuclide-specific solubility limits and partition coefficients for either oxidizing or reducing conditions. Diffusion coefficients are also radionuclide specific and assumed not dependent on redox conditions.

The basecase input parameter set does not consider the process or degradation of buffer/backfill material over time, because a bentonite buffer is assumed to be in a saturated, geochemically stable environment. Users may, however, implement time-dependent degradation in the buffer (zone 2) by (i) enabling degradation of the backfill via the Near Field component dashboard and (ii) defining input values for backfill initial failure time and backfill expected lifetime that are less than the model simulation period, and a fraction of cracked backfill that is greater than zero (these parameters are also available in the Near Field component dashboard). Doing so invokes the time-dependent degradation of the diffusive barrier capability of near-field zone 2, with an increasing total cracked volume fraction as backfill units degrade with time.

For calculating transport through the buffer/backfill in zone 2, inputs include height and width parameters to compute the cross-sectional area of the diffusive transport pathway and a length parameter to specify transport distance. For transport in zone 3, the distance is calculated based on the far-field fracture separation and a factor to account for uncertainty in the location of the waste package with respect to the nearest flowing fracture. The zone 3 diffusive transport calculation also includes a parameter to permit increasing or decreasing the diffusive cross-sectional area relative to that calculated for the zone-2 transport pathway. For fractured rock, the near-field flow factor is specified through the model dashboard to adjust the near-field flow velocity in proportion to the velocity in far-field Leg 1. By changing the near-field flow factor to a value greater than or less than the value of 1.0, the distribution specified in the input parameter will be overridden by the specified value.

4.3.4 Flexibility

Through careful selection or modification of input parameter sets and individual parameter values, the SOAR model has the flexibility to evaluate engineer barrier material properties, such as diffusion coefficients, diffusive area, and barrier thickness; evaluate geochemical properties, such as solubility constants and partitioning coefficients; and implicitly evaluate effects such as variability in pH, ionic strength, and pCO_2 by selecting input data sets for either reducing or oxidizing environments. The model also is capable of evaluating buffer degradation (zone 2) over time. Given the appropriate technical data, parameter values describing the buffer could be modified to represent materials other than bentonite (e.g., cement or other forms of clays).

The Near Field model component of the user interface dashboard allows users additional flexibility to evaluate alternative model concepts without the need to revise the input parameter distributions. Specifically, the dashboard provides users with the options to

- Bypass the near-field zone 2 diffusive barrier to examine cases not including a diffusive barrier around a waste package
- Disable advective releases
- Enable sorption in the zone 3 transition region
- Specify the input data value for volume of water inside the waste package (overrides default input value of 1.0)
- Specify the input data value for the near-field flow factor (overrides default input value of 1.0)
- Specify the fraction of change in the transport pathway cross section in zone 3 relative to zone 2 (overrides default input value of 1.0)

Users should avoid introducing conceptual inconsistencies when using the dashboard to override default parameter values. For example, selecting alternative values of the near-field flow factor would have no effect if the option to disable advective releases is also selected.

4.4 Far Field

4.4.1 Description

The Far Field model component of SOAR considers transport of released radionuclides within the natural-system component from the engineered barrier system to the biosphere. The Far Field model component specifically considers transport of radionuclides through geologic media, considering the effects of advection, diffusion, dispersion, decay, and sorption. The Far Field model component receives radionuclide releases from the Near Field model component and provides radionuclide releases to the Biosphere model component.

4.4.2 Model Implementation

The Far Field component considers a range of geologic media using a simplified representation for flow and transport. It has the flexibility to assign either a fracture-dominated or a matrix-dominated transport model to each of three transport segments (legs) within the same simulation. The first leg of the Far Field model component and zone 3 of the Near Field component use the same description for the disposal system host medium.

The Far Field component is based on the concept of one-dimensional advective-dispersive transport with equilibrium sorption to mineral grains and first-order decay of radionuclides, as defined next in Eq. (4-7). In this conceptual model, radionuclides released from the Near Field component are carried by water moving through the geologic media within a sequence of adjacent flow paths, conceptually referred to as stream-tube bundles. Each leg within the sequence is an effective stream tube that represents the many pathways in a complete bundle.

The parameters for the effective stream tube represent the average flow and transport parameters of the bundle.

The conceptual model is mathematically represented by the expression describing transport of a radionuclide species in the mobile zone

$$nR\frac{\partial c}{\partial t}=-\frac{Q}{A_{cs}}\frac{\partial c}{\partial x}+\left(\frac{\alpha Q}{A_{cs}}+D\right)\frac{\partial^2 c}{\partial x^2}+nR\left[-\lambda c+\sum_p c_p\lambda_p f_p S_p\left(\frac{WR_p}{W_pR}\right)\right]-\frac{F_{md}}{A_{cs}} \tag{4-7}$$

where n is effective porosity [unitless], R is the retardation factor [unitless], c is solute concentration [kg/m^3], Q is volumetric flow rate of water [m^3/yr], A_{cs} is cross-sectional area [m^2] perpendicular to flow direction, α is dispersivity [km], D is effective diffusivity [m^2/yr], λ is decay rate [1/yr], f is the fraction of the parent species that decays into the species [unitless], S is the stoichiometric ratio of moles produced per mole of parent [unitless], W is atomic weight [kg/mole], F_{md} represents diffusive mass flux per unit length of pathway [kg/yr/m] from water flowing in fractures (mobile zone) into the a stagnant water (immobile zone) within the adjacent rock matrix, t is time [yr], and x is distance along the pathway [m]. To make parameters dimensionally consistent, unit conversions are handled internally by the GoldSim software. A subscript p represents a parent species in a decay chain.

The flux into matrix diffusion zones is considered only for the conceptual model of fracture-dominated flow and is represented by

$$F_{md}=-\sum Pf_{im}D_{im}\left.\frac{\partial c}{\partial z}\right|_{z=0} \tag{4-8}$$

where P is the pathway perimeter [m], f_{im} is the fraction of the perimeter with matrix diffusion [unitless], D_{im} is effective diffusivity of the matrix diffusion zone [m^2/yr], and z is distance into the matrix diffusion zone [m].

From Eq. (4-8) it can be seen that the rate of diffusive transport into the stagnant matrix diffusion zone is controlled by the solute concentration gradient at the rock fracture–interface ($z = 0$) perpendicular to the flow direction. The time-dependent solute concentration within the matrix diffusion zone is calculated in GoldSim from

$$\frac{\partial c_{im}}{\partial t}=\left(\frac{D_{im}}{n_{im}R_{im}}\frac{\partial^2 c_{im}}{\partial z^2}\right)+\left[-\lambda c_{im}+\sum_p c_{im,p}\lambda_p f_p S_p\left(\frac{WR_{im,p}}{W_pR_{im}}\right)\right] \tag{4-9}$$

where symbols are the same as denoted for Eq. (4-7) except that the *im* subscript denotes the immobile region.

The retardation factor defines the transport velocity of radionuclides relative to the groundwater velocity. A retardation factor of 10, for example, indicates a transport velocity one-tenth that of groundwater.

The retardation factor for each radionuclide species is calculated as

$$R = 1 + \frac{\rho_b K_d}{\theta} \tag{4-10}$$

where ρ_b is the dry bulk density of the porous medium or rock matrix [kg/m^3], K_d is the radionuclide-specific equilibrium partition coefficient [m^3/kg], and θ is the saturated porosity of the porous medium or rock matrix [unitless]. For uniform flow in porous media, θ is equal to n in Eq.(4-7). For fracture flow with diffusion into a stagnant matrix zone, θ is equal to n_{im} in Eq. (4-9). Users are referred to GoldSim Technology Group, LLC (2010b) for a more thorough explanation of underlying solute transport modeling methods and assumptions used in the GoldSim pipe elements.

The Far Field component provides the capability to treat flow in each transport leg as either single porosity or dual porosity. A single-porosity flow leg represents uniform flow through a homogenous medium. A dual-porosity flow leg represents a heterogeneous system, such as fractured rock, where nearly all flow occurs in a small portion of the total porosity that can exchange mass by diffusion into the relatively stagnant water that occupies the remaining porosity of the unfractured rock mass. The type of model used and the associated parameters in the transport calculations depend on the medium selected. For calculating water flow rates in a single-porosity medium, volumetric water flux per unit area is calculated according to Darcy's Law by multiplying the hydraulic gradient by the bulk hydraulic conductivity. For flow in a dual-porosity system fractured medium, Darcy's Law is also used to represent volumetric water flux per unit area. In this case, however, two sampled parameters—effective fracture aperture and average flowing fracture separation—are used to calculate an equivalent hydraulic conductivity using the cubic law for flow between parallel plates. The cubic law relates average volumetric flux to the cube of the aperture. The effective fracture aperture is the aperture that yields the same average volumetric flux as the actual aperture distribution. The fracture length density describes the total length of flowing fractures per unit rock area in the plane perpendicular to flow direction. Effective porosity is assumed to be the product of effective equivalent or representative aperture and fracture length density. The fracture length density and perimeter for exchange with the matrix diffusion zones are calculated using the conceptual model of parallel flowing fractures, each extending the height of the stream-tube bundle and separated by an average distance. With this conceptual model, the fracture length density is the inverse of the average separation distance.

Some inherent assumptions and key processes represented by the previous computational approach include the following:

- Flow in fractures and porous media is assumed slow and laminar, such that Darcy's Law (i.e., flow rate is proportional to hydraulic gradient) is a valid approximation and turbulent flow effects can be neglected.

- Longitudinal contaminant dispersion during transport that results from variability in flow velocities within adjacent flow pathways is assumed to be proportional to average water velocity, with a proportionality constant called dispersivity. The resulting smearing of transport times caused by dispersion is assumed to be dominant such that the effect of molecular diffusion can be ignored. The dispersion coefficient (α) is assumed to be scale dependent and is calculated as a fraction of the transport path length (e.g., 10 percent in the basecase parameter set).

- When fractured rock is selected as the geologic medium for a transport leg, the model considers the flowing fractures to be a mobile zone with adjacent immobile zones representing both the low-permeability rock matrix and any nonflowing fractures. The GoldSim software is capable of representing up to three different geometric configurations for the interface between mobile and immobile zones. These geometries include (i) a slab (diffusive area is constant with distance into the matrix), (ii) a sphere (diffusive area decreases with distance into the matrix, like a matrix block between bounding fractures), and (iii) a slot (diffusive area increases exponentially with distance into the matrix). Each immobile zone may occupy a fraction of the fracture perimeter and extend halfway to the next flowing fracture. The default setup for the Far Field component calculates matrix diffusion flux using the slab geometry with no "skin zone" enabled (skin zone refers to a thin zone at the fracture surface that permits instantaneous sorption).

- Some radionuclides can be sequestered onto the surface of solid particles for long periods of time by sorption. The Far Field component represents sorption using the assumption that the ratio of sorbed radionuclides to dissolved radionuclide concentration rapidly obtains a single fixed value regardless of concentration (i.e., equilibrium linear sorption). This fixed ratio equals the product of the partition coefficient, K_d, and the dry density, ρ_b. Conceptually, sorption describes electrochemical attachment of a radionuclide molecule to one of many attachment sites on the solid surface. For some radionuclides, the partition coefficient may differ by orders of magnitude with different values of pH, salinity, redox potential, dissolved-species concentrations, and specific surface area (surface area per unit volume). The current version of SOAR only considers sorption to fixed static surfaces (i.e., colloidal transport is not included). When a porous medium is selected for a transport leg, sorption is assumed to occur throughout the porous medium. When a fractured medium is selected, sorption is assumed to occur only within the stagnant rock matrix.

- The transport model does not account for precipitation or dissolution. Each radionuclide is assumed to have concentrations no greater than the ambient solubility limit.

4.4.3 Default Parameters

A complete list of default parameter values, distribution types, and technical bases for the Far Field component is provided in Appendix A, Table A–4. Parameter sets were developed for three types of transport media: fractured rock, unconsolidated sediments, and porous clay. Radionuclide-specific sorption coefficients (K_d), bulk density (ρ_b), effective porosity (θ), and matrix diffusion coefficients (D_{im}) were selected based on literature reviews of laboratory and field testing from domestic and international geologic disposal system programs. Properties for fracture-dominated flow systems were selected to be consistent with flow in granitic rock (SKB, 2006). Properties for unconsolidated sediments were based on studies of alluvium for the Yucca Mountain project (DOE, 2008). Properties for the porous clay medium are based on a variety of sources for properties of clays suitable for geologic disposal sites (NEA, 2005; Nirex Limited United Kingdom, 2003; SKB, 1997).

4.4.4 Flexibility

With appropriate selection or modification of input parameters such as radionuclide distribution coefficients and hydraulic conductivity, the Far Field component is capable of representing flow and transport through a wide range of porous or fracture-dominated natural media. For example, with modification of these parameters, one could represent transport through basalt or sandstone. The Far Field component provides default parameters for each equivalent stream tube as described in the preceding list of assumptions. The default parameters for porous medium legs are representative of oxidizing conditions in typical alluvium. The default parameters for fractured medium legs are representative of reducing conditions in typical fractured granite.

The Far Field component of the user interface dashboard allows users additional flexibility to evaluate alternative model concepts without the need to revise the input parameter distributions. Specifically, the dashboard provides users with the options to

- Select the conceptual models for flow (fracture dominated or matrix dominated) and geochemical environment (oxic or anoxic) the combination of these two conditions affects the selection of radionuclide sorption coefficients used in the transport calculations

- Specify the transport path length for each of the three transport legs

- Specify the effective flow porosity in each of the transport legs

- Specify the hydraulic conductivity in each of the transport legs

4.5 Biosphere

4.5.1 Description

The Biosphere model component converts radionuclide mass arrival from the Far Field model component into radiological dose to a person (receptor) in the biosphere. In this version of the performance assessment model, biosphere considerations were simplified to only address the drinking water pathway. No other dose pathways are considered. Integrated radionuclide release is also calculated to provide a second metric of system performance.

4.5.2 Model Implementation

The Biosphere component computes radiological dose in the following manner

$$E = \sum_i m_i \times \frac{CF}{Q} \times a_i \times I \times d_i \times C^* \qquad (4\text{-}11)$$

where E [mrem/yr] is the annual effective dose; m_i [g/yr] is the mass arrival rates from the Far Field component for radionuclide I; CF [unitless] is the capture fraction; Q [acre-ft/yr] is the water flow rate to the biosphere; a_i [Ci/g] is the specific activity for radionuclide I; I [L/yr]is the water consumption rate; d_i [Sv/Bq] is the dose coefficient for ingestion of radionuclide; I and C^* is the product of unit conversions for volume [acre-ft/L], activity [Bq/Ci], and dose equivalent [mrem/Sv].

The calculation of radiological dose involves the following steps in the model. Several steps include internal unit conversions.

- Radionuclide mass concentrations in water (g/L) are calculated by multiplying radionuclide mass arrival rates (g/yr) by a capture fraction (unitless) and dividing by the annual water flow rate to the biosphere (acre-ft/yr). The mass arrival rates for each radionuclide are passed from the Far Field component to the Biosphere component.

- Radionuclide mass concentrations in water are converted to radionuclide activity concentrations in water (Ci/L). This conversion applies internal specific activity definitions for individual radionuclide species.
- Annual radionuclide dose to the receptor is calculated by multiplying the radionuclide activity concentration in water with the product of annual water consumption rate (L/yr) and the radionuclide dose coefficient for ingestion (Sv/Bq). Doses are calculated for ingestion of drinking water only.

- The total annual dose (mrem/yr) is calculated by summing the annual dose contributions from the individual radionuclides. Individual radionuclide doses and the total dose from all radionuclides are computed. Doses to individual organs are not calculated.

Radionuclide and total dose results are weighted by event probability for disruptive events (see Section 4.6, Disruptive Events). Probability weighting of doses is not performed for the waste package failure rate or no disruptive event options. Integrated release is calculated as described in 40 CFR Part 191, Appendix A, Subpart B, Table 1. This calculation in SOAR assumes that the initial inventory falls into the category of 40 CFR Part 191, Subpart B, Table 1, Note 1(a), where the waste form is based on a burnup rate of 25,000–40,000 MWd/MTHM.

4.5.3 Default Parameters

The Biosphere component includes four input parameters: WaterFlowToBiosphere, Capture_Fraction_Used, Water_Consumption_Rate, and Ingestion_Dose_Coefficient. The default parameter values, distribution types, and technical bases for the default parameters of the Biosphere component are listed in Appendix A, Table A–5.

Parameter distributions for sampling the water flow rate to the biosphere and amount of contaminated water the receptor consumed were selected to account for variability and uncertainty in regional irrigation practices, community water usage, and individual habits regarding water consumption from a well or natural surface-water source (e.g., spring). Constant values are used for the other biosphere parameters.

The WaterFlowToBiosphere parameter represents the water flow rate to the biosphere used to calculate radionuclide concentrations in water available at the interface between the far field and the biosphere. Irrigation practices were used to establish groundwater usage for a small farming community, consisting of four farms of average size with respect to number of acres irrigated by groundwater. The parameter distribution accounts for variability in groundwater usage based on different water resource regions of the contiguous 48 states. The data source for this parameter value is U.S. Department of Agriculture (2010, Table 11).

The Capture_Fraction_Used parameter modifies the concentration of radionuclides in water and accounts for the fraction of water accessible to the biosphere that is contaminated and/or the fraction of total radionuclide mass from the far field that is transferred to the biosphere. There is no specific data source. The initial value of unity for this parameter does not change the concentration calculation and implies that all radionuclide mass transported to the end of the Far Field is completely transferred to the Biosphere.

The Water_Consumption_Rate parameter represents the population-averaged consumption rate of community water for adults in the United States. The data source for this parameter value is the U.S. Environmental Protection Agency (2004, Table A1, Appendix E, p. E-4). Because the selected source data accounted for both direct (water ingested as a beverage) and indirect (water added to foods and beverages during final preparation) intake, the distribution was based on reported survey data up to the 95th percentile.

The Ingestion_Dose_Coefficient parameter provides the radiological dose to an adult from the ingestion of a unit radionuclide activity. The ingestion dose coefficient parameter is implemented as a tabular array with separate values for each radionuclide. The data source for these parameter values is the International Commission on Radiological Protection (1996, Table A.1).

4.5.4 Flexibility

No particular site has been selected or assumed for geologic disposal from which to model the biosphere in this flexible performance assessment model. As described in the default parameter section, a generic parameter distribution for water flow to the biosphere was determined from data on groundwater usage for irrigation. Alterative distributions for this parameter could be specified to represent water practices for a specific region or regions as candidate disposal sites.

A capture fraction parameter adds flexibility in the biosphere for calculating radionuclide concentrations in water that are representative of the annual intake of contamination by an average member of a critical group. The parameter can be used to account for the situation where water access and usage by a nearby community include water from other sources that is not contaminated with radionuclides. The parameter can also account for the incomplete transfer of radionuclides from the far field to the biosphere (e.g., if plume dimensions exceed well capture zones).

4.6 Disruptive Events

4.6.1 Description

The Disruptive Events model component of SOAR (i) considers additional waste package failure mechanisms not included in the Waste Package model component, (ii) includes three additional waste package failure abstractions, and (iii) receives no inputs from other SOAR components. Additionally, the Disruptive Events model component provides waste package failure times to the Waste Form model component to initiate computations of waste form degradation for each failed waste package, breached area per failed waste package, and a dose modification factor to the Biosphere component based on event probability.

4.6.2 Model Implementation

The Disruptive Events component considers three waste package failure abstractions: a single failure event, multiple failure events, or a defined waste package failure rate (Figure 4-2). Only one of these three options can be used within a simulation. In Section 4.2, additional maximum waste package breach fraction that can range from 0 to 1 and is assumed to be uniformly distributed. The value used is sampled from the user-defined distribution once per realization. The duration of the assumed mechanism leading to waste package failure is also user defined. The user can control the starting time and the end time for which the failure mechanism is active. No waste packages are assumed to fail once the failure mechanism is inactive.

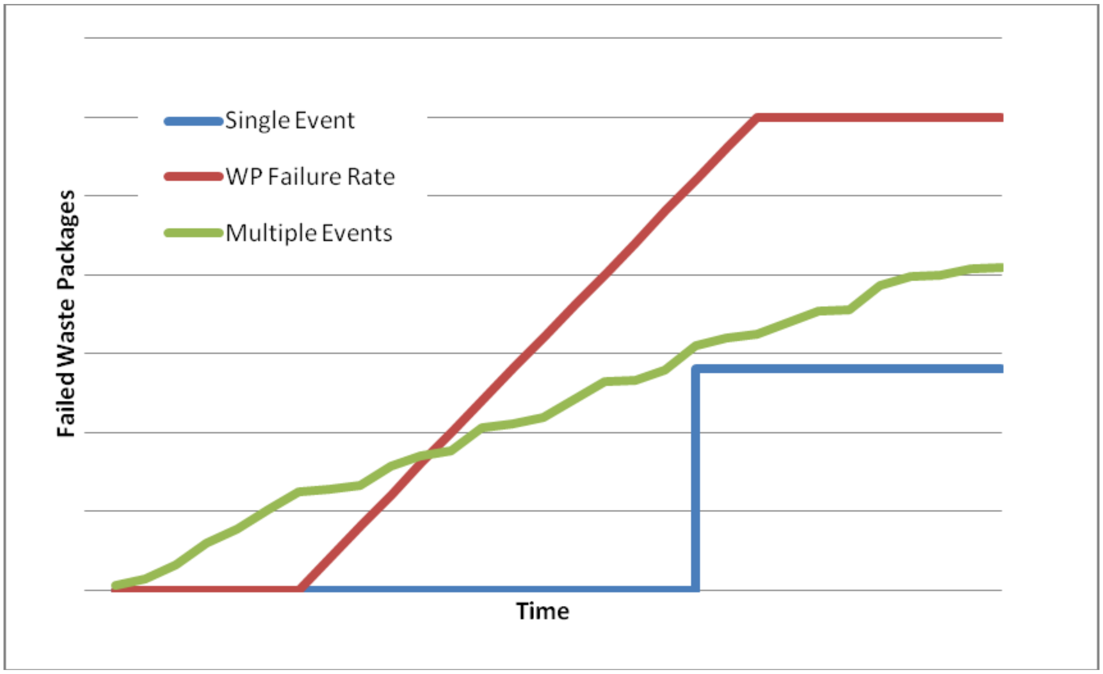

Figure 4-2. Characteristic Waste Package Failure Curves for the Three Abstractions Implemented in the Disruptive Events Model Component

Single Failure Event Abstraction

The single failure event is assumed to occur once in each realization at a random time. The single failure event abstraction requires three inputs for implementation in SOAR: the fraction of waste packages damaged, the extent of damage, and the probability for the event to occur.

The user defines a minimum and maximum fraction of waste packages damaged ranging from 0 to 1. The fraction of failed waste packages is assumed to follow a uniform distribution. One value is sampled per realization from the user-defined distribution.

The waste package damage is defined as the fraction of the waste package surface breached that no longer provides a barrier to radionuclide release. The user defines a minimum and maximum waste package breach fraction that can range from 0 to 1. The breach fraction is assumed to follow a uniform distribution. The value is sampled from a user-defined distribution, once per realization.

The probability of the event occurring also defined by the user, is used to approximate the effect of low probability events on radionuclide dose. The event probability is multiplied by the simulation duration to obtain a dose modification factor. This modification factor is applied to the total dose and radionuclide dose to obtain probability-weighted versions of these results. The modification factor is not applied to other intermediate results. Also note that the dose modification factor is a linear approximation, which is valid for low recurrence rates. The approximation error increases as the probability of the event for a given realization approaches one. The approximation is reasonable if the product of the recurrence rate (e.g., 10^{-7} /yr^{-1}) and the simulation time (e.g., 10^6 yr) is less than 0.1.

Multiple Failure Event Abstraction

The multiple failure event abstraction conceptually models multiple disruptive (failure) events. The events are assumed to occur randomly via a Poisson process. The multiple failure event abstraction requires three inputs for implementation in SOAR: the event frequency, the probability of damage for a given event, and the damage area for a given event.

The user defines the minimum and maximum event recurrence rates to define a uniform distribution. SOAR utilizes a Timed Event element to generate each event that has the potential to impact the waste packages. These events are generated following a Poisson process. The recurrence rate (from which the event intensity is derived) is sampled from the former uniform distribution. The range of recurrence rates considered in SOAR ranges from 10^{-4} yr^{-1} – 10^{-8} yr^{-1}. For each order of magnitude change in recurrence rate, the user can define a fraction of waste packages that are assumed to fail and the extent of waste package surface damage or breach area to create a hazard curve. Values for the event impact (i.e., the number of waste packages affected by an event of a given sampled recurrence rate) are interpolated from the user-defined hazard curve. Events with a recurrence rate greater than 10^{-4} yr^{-1} are assumed to have no impact on waste package integrity, while events of less than 10^{-8} yr^{-1} are assumed to have the same impact as the 10^{-8} yr^{-1} recurrence rate events. As an example, for seismic events that occur with a frequency of 1 in 10,000 years, or more often, are assumed to have peak ground velocities and peak ground accelerations not causing major damage to the waste packages. Events with a frequency of 1 in 100 million years (or even less frequent) are assumed to be destructive and damage the majority of the waste packages. In the model, consequences of such high intensity events are restricted to waste package damage. However, extreme events could have other large effects on the system, such as changes to the landscape and water flow paths. Other potential alternative effects are not presently included in the model.

Waste Package Breached Area

The waste package breached area from the three additional waste package failure abstractions described previously is combined with the breached area from the corrosion process modeled in the Waste Package model component described in Section 4.2. See Section 4.2.2 for a description of the computation of the combined breached area, including waste package failure by corrosion and disruptive events.

GoldSim and Waste Package Counting

As previously stated, only one of the three disruptive event alternatives can be executed in a simulation. In addition, a simulation can include waste package failure due to corrosion. The Corrosion Model component and the Disruptive Events model component output the fraction (ranging from 0 to 1) of waste packages failed due to corrosion and to the disruptive events, respectively. These fractions are input to GoldSim source term elements to compute total radionuclide releases from the EBS. The GoldSim source term computes the total number of waste packages failed by combining the failure fractions under the assumption that these fractions are independent. For example, if the fraction of waste packages failed by corrosion is 0.5 and the fraction of waste packaged failed by disruptive events is 0.7, the total fraction of waste packages failed is 0.5 + 0.7 - 0.5 × 0.7 = 0.85. The fraction of waste packages that fail due to corrosion and the disruptive event is 0.5 × 0.7 = 0.35. The fraction of waste packages that fail due to corrosion only is 0.5 - 0.35 = 0.15. The fraction of waste packages that fail due to the disruptive events (and not due to corrosion) is 0.7 - 0.35 = 0.35. By adding these last three numbers, 0.35 + 0.15 + 0.35 = 0.85, which is another way to compute the fraction of waste packages failed due to either corrosion or disruptive events. The GoldSim source term element performs these computations automatically and generalizes these computations for the case when multiple (two or more) independent failure modes are considered.

4.6.3 Default Parameters

The default parameters for the Disruptive Events model component were arbitrarily chosen to cover a broad range of values. As such, no values have been documented in Appendix A or the SOAR database.

4.6.4 Flexibility

With appropriate selection or modification of input parameters, such as event recurrence rate, waste package damaged fraction, and breached area fraction, the Disruptive Events component is intended to represent a variety of approximations of disruptive events and other failure mechanisms.

The Disruptive Events component of the user interface dashboard allows users additional flexibility to evaluate alternative model concepts without the need to revise the input parameter distributions. Specifically, the dashboard provides users with the options to

- Select and activate one of the additional waste package failure abstractions described in this section. (Specific inputs were discussed earlier in Section 4.6.2.)

- Specify the damage area fraction for the waste packages.

5 MODEL CONFIDENCE

In this section, activities aimed at enhancing confidence in the models implemented in Scoping of Options and Analyzing Risk (SOAR) are discussed. The model review and testing conducted to gain model confidence are summarized in the following bullets.

- All GoldSim model elements (e.g., data elements, mixing cells, pipe pathways, selectors, results elements) were visually inspected to ensure correct computations and algorithms were implemented, correct units were used, and inputs and outputs connected to the correct elements. For most model elements, text descriptions were added to help users understand the purpose of the element.

- Individual realizations were run using high and low input parameter values, and results were inspected to ensure intermediate outputs and system-level response were reasonable. For example, the model was run using the highest and lowest waste form degradation rate and results compared against the expectation that higher waste form degradation rates resulted in proportionally higher release.

- Different combinations of waste form, waste package material, and geochemical environment were run, and intermediate-level and system-level outputs were evaluated to verify that the model selected the correct inputs and computational algorithms appropriate to the model settings.

- The initial inventory of radionuclides was varied from very small to very large values to check a proportional output response.

- In addition to these initial testing efforts, developers at the U.S. Nuclear Regulatory Commission (NRC) and Center for Nuclear Waste Regulatory Analyses (CNWRA®) carried out a more detailed verification effort. The effort included development of a number of test plans, test reports, and a status spreadsheet and focused on testing all of the major model components.

The SOAR code was developed with the GoldSim language, which is an icon-based, high-level programming language. As such, it does not lend itself to traditional verification techniques associated with sequential languages (e.g., FORTRAN, C++) frequently used for modeling physical phenomena. However, it can automatically perform many of the checks required for a sequential language. For example, GoldSim can automatically check for proper parameter types, consistent units of physical quantities, and meaningful syntax and establish a proper connection between functional elements. Given the automatic availability of these features, a number of verification activities focused on performing visual inspections of equations in the GoldSim elements, determining their logical relationship to other programming elements, and analyzing results. In general, performed tests relied on qualitative comparison of results with respect to expected values.

Teams of analysts developed the multidiscipline models, or model components, in SOAR. When each team member is able to work on any of the model components, there is an opportunity to check the work of other team members. Many self-checks of this nature were performed during the development of the code, including visual inspection of equations and review of the logical structure of each model component. A first level of confidence in the code was attained during development using this self-checking technique. Also, the availability of intermediate values and outputs enabled the inspection of the output response of each component to changes in input values.

A model that represents a physical process, with the associated uncertainties, requires the ability to vary the value of model parameters to represent ranges of possible conditions. Flexible parameter values are also required to investigate relevant scenarios that may differ from base models. Parameters are also used to implement specific features of the model or otherwise control the operation of the model during execution. During the model development, a number of input parameters were revised. In general, modification of input parameters in a model component of SOAR does not affect the functionality of another independent model component. Therefore, in general, tests on a particular model component were not repeated when input parameters for other model components changed. Numerous preliminary input parameter values were used in development testing. Documented selection of input parameter values are supplied with the release of Version 1.0.

During the code development process, repeated tests were commonly executed by inputting many different values for the relevant parameters to check the behavior of the component being constructed. This process frequently used the dashboards to enter the new values, with the intention to test the dashboard interface, as well as the corresponding model component. In this way the mechanics of the parameter entry dialog and the propagation of the parameter value to the model components were evaluated. The dashboard interface also enabled the convenient testing of parameter minimum and maximum value limits. During the development of the code, no formal documentation was prepared to establish agreement with external calculations; however, the output was continually checked to ensure self-consistency. Qualitative testing was also performed on input values and mode selectors available in dashboards.

The SOAR model has the ability to consider up to four different waste form types. While the model components for each waste form type share similarities, separate independent tests were performed for each type. Integrated tests were also performed to test the capability of the model to handle cases with simultaneous presence of multiple waste forms. These kinds of tests were performed during the development of the Waste Form model component and during formal testing phases.

Once the model was considered to be relatively mature, formal verification tests were implemented. These formal verification tests were mostly high-level tests that focused on one specific model component at a time. Each test was documented in a test report summary. These formal tests exercised the operation of model component dashboards, input parameter values, and switches. These tests included the qualitative analysis of intermediate output values by the particular model component. By studying the qualitative trends of outputs, or changes in outputs in response to changes in inputs, a conclusion was attained on whether an aspect of a model was appropriately implemented. The SOAR model was revised when necessary to address issues identified during the formal testing phase.

Formal tests were organized into six groups, each identified with one of the following two letter abbreviations:

- Waste Form (WF)
- Waste Package (WP)
- Near Field (NF)
- Far Field (FF)

- Dashboard (DB)
- Disruptive Events (DE)

Each group tested one or more aspects of the target component. To isolate the aspect/parameter for a test, it was frequently necessary to configure other parameters or switches in a way that would disable parts of the model that could potentially impose conditions that would influence the results more than the aspect being tested. The testing of a particular aspect was, in general, compared to a reference run and to several runs with different inputs than the reference run.

Documentation for the verification effort was maintained as Microsoft® Word® and Excel® files on a drive shared by NRC and CNWRA developers. The documentation consisted of test plans, test reports, and a status spreadsheet. The test plan identified the test objective, specified the criteria for a successful test, and was generated prior to each test. The results of the test were documented in a test report summary that displayed the data in text or chart form as output by SOAR, as well as the status of the test.

Exhaustive testing of modeling software can be time consuming and difficult to design. The design of the tests performed to verify the SOAR model balanced time available by testers with the level of confidence desired in the code performance (taking into account that SOAR is intended as a generic tool for scoping computations). This resulted in the execution of a limited number of tests. Further tests for internal consistency could be aimed at database value propagation, convergence of statistical results as a function of increasing number of realizations, and dependence of results on timesteps. Quantitative tests can be defined; for example, the SOAR model could be compared to external codes that perform a subset of similar calculations. This type of test is time consuming to implement because inputs must be identical for results to match, the model or code used as comparison must be thoroughly understood, and SOAR and the comparison code must be adjusted to yield comparable outputs. Later development work will analyze the feasibility of performing this kind of benchmarking testing.

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APPENDIX A
DEFAULT INPUT PARAMETERS

Table A–1. Default Parameters for SOAR Waste Form Model Component			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
DegRate_HLW_Ceramic	HLW Ceramic Waste Form Degradation Rate (yr^{-1})	Log-uniform 1.50E-08, 2.00E-06	BSC (2004a); Reeve, et al. (1989); Vance, et al. (1997); Wang (2009)
DegRate_HLW_Glass	HLW Glass Waste Form Degradation Rate (yr^{-1})	Log-uniform 1.50E-06, 2.00E-04	BSC (2004a); Iseghem (2007)
DegRate_sMOX_Combined	sMOX Waste Form Degradation Rate (yr^{-1})	Log-uniform 9.00E-07, 6.00E-04	Ebert, et al. (2002); Wang (2009)
DegRate_sMOX_Oxidizing	sMOX Waste Form Degradation Rate (yr^{-1})	Log-uniform 3.00E-05, 6.00E-04	Ebert, et al. (2002); Wang (2009)
DegRate_sMOX_Reducing	sMOX Waste Form Degradation Rate (yr^{-1})	Log-uniform 9.00E-07, 2.00E-05	Ebert, et al. (2002); Wang (2009)
DegRate_SNF_Combined	CSNF Waste Form Degradation Rate (yr^{-1})	Log-uniform 9.00E-07, 6.00E-04	Leslie, et al. (2007); NRC (2008); Shoesmith (2000)
DegRate_SNF_Oxidizing	SNF Waste Form Degradation Rate (yr^{-1})	Log-uniform 3.00E-05, 6.00E-04	Leslie, et al. (2007); NRC (2008); Shoesmith (2000)
DegRate_SNF_Reducing	SNF Waste Form Degradation Rate (yr^{-1})	Log-uniform 9.00E-07, 2.00E-05	Leslie, et al. (2007); NRC (2008); Shoesmith (2000)

Table A–1. Default Parameters for SOAR Waste Form Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
HLWc_Radionuclide_Mass_WP	HLW Ceramic Radionuclide Inventory (g) [C14, Cs135, I129, Np237, Pu238, Pu239, Pu240, Pu242, Se79, Tc99, U232, U233, U234, U235, U236, U238]	Constant-vector [0.00E+00,7.65E+02, 1.02E+02, 1.05E+02, 1.69E+00, 1.30E+04, 3.04E+02, 5.84E+00, 0.00E+00, 0.00E+00, 8.15E-06, 1.46E-03, 3.06E+01, 2.73E+03, 6.51E+01, 1.46E+04]	SNL (2007) Tipton (2010) The inventories for Pu-241 and Am-241 are added to the initial inventory of Np-237 to account for ingrowth.
HLWg_Inventory_per WP	HLW Glass Radionuclide Inventory (g) [C14, Cs135, I129, Np237, Pu238, Pu239, Pu240, Pu242, Se79, Tc99, U232, U233, U234, U235, U236, U238]	Constant-vector [2.91E-01, 9.47E+02, 9.36E+01, 5.06E+02, 5.31E+01, 3.43E+02, 3.86E+01, 5.44E+00, 1.36E+03, 1.47E-03, 9.39E+00, 1.79E+01, 3.07E+02, 5.69E+01, 1.41E+05]	(DOE, 2009b) Tipton (2010) The representative inventory for HLW Glass is derived based upon values taken from DOE (2009b). Because there is uncertainty on future inventories for glass waste, a representative bounding glass was created based on DOE (2009b, Table 1.5.1-21, pp. 1.5.1-167 through 1.5.1-171). The representative glass waste form for the current approach was derived as a composition of the four glass waste forms (Hanford, Savannah River Site, West Valley, and Idaho) by selecting the maximum radionuclide inventories from the four types presented in DOE (2009b, Table 1.5.1-21. Additionally, the inventories for Pu-241 and Am-241 were added to the initial inventory of Np-237 to account for ingrowth.

Table A–1. Default Parameters for SOAR Waste Form Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
sMOX_Inventory_2035_Default	sMOX Radionuclide Inventory (g) [C14, Cs135, I129, Np237, Pu238, Pu239, Pu240, Pu242, Se79, Tc99, U232, U233, U234, U235, U236, U238]	Constant-vector [2.58E+00, 7.17E+03, 3.09E+03, 4.64E+04, 1.50E+03, 1.03E+05, 7.26E+04, 1.84E+04, 9.98E+03, 1.01E-03, 2.33E-03, 9.13E+01, 5.62E+03, 2.23E+03, 8.19E+06]	SNL (2007) Tipton (2010) The inventories for Pu-241 and Am-241 were added to the initial inventory of Np-237 to account for ingrowth.
SNF_Inventory_2010_default	CSNF Radionuclide Inventory (g) [C14, Cs135, I129, Np237, Pu238, Pu239, Pu240, Pu242, Se79, Tc99, U232, U233, U234, U235, U236, U238]	Constant-vector [1.35E+00, 4.36E+03, 1.73E+03, 1.54E+04, 1.52E+03, 4.32E+04, 2.05E+04, 5.28E+03, 7.55E+03, 1.02E-02, 5.76E-02, 1.75E+03, 6.26E+04, 3.84E+04, 7.82E+06]	DOE (2009b) Tipton (2010) Inventories for Pu-241 and Am-241 were added to the initial inventory of Np-237 to account for ingrowth.
UnboundFraction_sMOX_C14	C14 Unbound Fraction for sMOX (Instant Release Fraction from GAP/grain inventory)	Constant 0.1	Jain, et al. (2004); Tipton (2010)
UnboundFraction_sMOX_Cs135	Cs135 Unbound Fraction for sMOX (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0088, 0.025, 0.058	Leslie, et al. (2007); Tipton (2010)

Table A–1. Default Parameters for SOAR Waste Form Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
UnboundFraction_sMOX_I129	I129 Unbound Fraction for sMOX (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0054, 0.11, 0.32	Leslie, et al. (2007); Tipton (2010)
UnboundFraction_sMOX_Se79	Se79 Unbound Fraction for sMOX (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0088, 0.025, 0.058	Leslie, et al. (2007); Tipton (2010)
UnboundFraction_sMOX_Tc99	Tc99 Unbound Fraction for MOX (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0005, 0.0013, 0.0028	Leslie, et al. (2007); Tipton (2010)
UnboundFraction_SNF_C14	C14 Unbound fraction for SNF (Instant Release Fraction from GAP/grain inventory)	Constant 0.1	Jain, et al. (2004); Tipton (2010)
UnboundFraction_SNF_Cs135	Cs135 Unbound Fraction for SNF (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0088, 0.025, 0.058	Leslie, et al. (2007); Tipton (2010)

Table A–1. Default Parameters for SOAR Waste Form Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
UnboundFraction_SNF_I129	I129 Unbound Fraction for SNF (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0054, 0.11, 0.32	Leslie, et al. (2007); Tipton (2010)
UnboundFraction_SNF_Se79	Se79 Unbound Fraction for SNF (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0088, 0.025, 0.058	Leslie, et al. (2007); Tipton (2010)
UnboundFraction_SNF_Tc99	Tc99 Unbound Fraction for SNF (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0005, 0.0013, 0.0028	Leslie, et al. (2007); Tipton (2010)

Table A–2. Default Parameters for SOAR Waste Package Model Component			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
CS_GC_Anox_High	Carbon steel, high bound for the corrosion rate, reducing medium (μm/yr)	Constant 10	Pitting corrosion is not obvious in reducing condition. A pitting enhancement factor of 1 was added to the general corrosion rates in reducing condition for the current code. Bennett and Gens (2008); Johnson and King (2008); Feron, et al. (2008); Ahn and Soo (1995); Ahn and Leslie (1998); Taniguchi, et al. (2004); Foct, et al. (2004); Kursten, et al. (2004a,b); Foct and Gras (2003)
CS_GC_Anox_Low	Carbon steel, low bound for the corrosion rate, reducing medium (μm/yr)	Constant 0.1	Pitting corrosion is not obvious in reducing condition. A pitting enhancement factor of 1 was added to the general corrosion rates in reducing condition for the current code. References are the same as previous.
CS_GC_Ox_High	Carbon steel, high bound for the corrosion rate, oxidizing medium (μm/yr)	Constant 150	Literature reports pitting enhancement factor of 1–3. A pitting enhancement factor of 1.5 was added to the general corrosion rates in oxidizing condition for the current code. References are the same as previous.
CS_GC_Ox_Low	Carbon steel, low bound for the corrosion rate, oxidizing medium (μm/yr)	Constant 15	Literature reports pitting enhancement factor of 1–3. A pitting enhancement factor of 1.5 was added to the general corrosion rates in oxidizing condition for the current code. References are the same as previous.
Cu_GC_Anox_High	Copper, high bound for the corrosion rate reducing medium. (μm/yr)	Constant 0.02	A pitting enhancement factor of 5 was considered. Uncertainty remains on sulfate concentration. If sulfate concentration could be higher than what was used in the Swedish report, another enhancement factor should be considered. Wersin, et al. (1994)

Table A–2. Default Parameters for SOAR Waste Package Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Cu_GC_Anox_Low	Copper, low bound for the corrosion rate, reducing medium (μm/yr)	Constant 0.004	A pitting enhancement factor of 5 was considered. If sulfate concentration could be higher than what was used in the Swedish report, another enhancement factor should be considered. Wersin, et al. (1994)
Cu_GC_Ox_High	Copper, high bound for the corrosion rate, oxidizing medium (μm/yr)	Constant 7	A pitting enhancement factor of 100 was considered. If sulfate concentration could be higher than what used in the Swedish report, another enhancement factor should be considered. Wersin, et al. (1994)
Cu_GC_Ox_Low	Copper, low bound for the corrosion rate, oxidizing medium (μm/yr)	Constant 0.04	A pitting enhancement factor of 5 was considered. If sulfate concentration could be higher than what was used in the Swedish report, another enhancement factor should be considered. Wersin, et al. (1994)
LC_FailureTime_Period_I	Failure time by LC for the early Period I (assumed that all LC affected WPs fail at the same time) (yr)	Log-uniform 30, 280	Period I is used to define an early period over which the WP may experience localized corrosion. In a repository located in reducing media, a transient oxidizing period could develop before return to the long-term reducing conditions, over which the chance for localized corrosion is higher. Taniguchi, et al. (2004) reported that for a geological disposal repository of high-level radioactive waste in Japan, the period until environmental condition return from oxidizing to reducing is expected to be less than 100 years. Wersin, et al. (1994) reported a maximum period of 280 years for oxidizing condition. Taniguchi, et al. (2004) reported the oxidizing period is 30 years. Based on these data, it is assumed that localized corrosion could initiate during the oxidizing period, up to 280 years.

Table A–2. Default Parameters for SOAR Waste Package Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
LC_FailureTime_Period_II	Failure time by LC for the late Period II (assumed that all LC affected WPs fail at the same time) (yr)	Log-uniform 280, 1.00E+05	Period II is used to define a late period over which the WP may experience localized corrosion. For a repository located in reducing media, this period II time parameter defines the time at which the WP may experience localized corrosion after the return of the repository to reducing conditions.
LC_FractionAreaBreached	Fraction of WP area breached by LC (unitless)	Log-triangular 0.001, 0.1216	According to literature information on stainless steel pitting corrosion in chloride solution, the maximum breach area for the stainless steel waste packages should not exceed 5 percent of the total area. Considering that the waste package may be in contact with buffer material and the buffer material may degrade with time to form fractures, stainless steel crevice corrosion is also considered possible, especially for repository in oxidizing media. To support rate of metal dissolution reactions on anodic sites, it is conservatively estimated that cathodic area needs to be at least five times that of anodic sites. This is because both oxygen and water reduction reactions occur at much slower rates compared to metal dissolution reactions at anodic sites. Considering this, an upper bound of 20 percent is used. A log-triangular distribution is considered.
SS_GC_Anox_High	Stainless steel, high bound for the corrosion rate, reducing medium (μm/yr)	Constant 0.1	Based on corrosion studies performed in cementitious backfill material, Kursten, et al. (2004b) summarized that the long-term anoxic corrosion rate of stainless steel at all repository temperatures is <0.01 μm/yr. Based on *in-situ* corrosion studies relevant to the Belgian disposal concept in clay, Kursten et al. (2004b) summarized that the maximum corrosion rate was 0.15 μm/yr at 170 °C [338 °F] with most of the corrosion rates less than 0.1 μm/yr. Based on these limited data in anoxic condition, it is reasonable to assume that the maximum corrosion rate is 0.1 μm/yr [3.9 μin/yr]. A distribution skewing toward the lower end is preferred.

Table A–2. Default Parameters for SOAR Waste Package Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
SS_GC_Anox_Low	Stainless steel, low bound for the corrosion rate, reducing medium (μm/yr)	Constant 0.003	Based on Kursten, et al. (2004b, Table 4-34). This low rate is also near the resolution limit of the weight loss analysis method to determine corrosion rate.
SS_GC_Ox_High	Stainless steel, high bound for the corrosion rate, oxidizing medium (μm/yr)	Constant 3	Select Switch_GC_DistributionType=1(normal), Switch_GC_DistributionScale=1(log); i.e., log-normal distribution in corrosion rates. Based on corrosion studies performed in cementitious backfill material summarized in Kursten, et al. (2004b, Table 4-54 and Figure 4-72). Tests were conducted at pH of 1.9–13 and temperatures of 30–80°C [86–176 °F]. The corrosion rate increased with decreasing pH. At pH of 4 and 80 °C [176 °F], the corrosion rate was 2.6 μm/yr [102.4 μin/yr]. Based on other data from international geological repository programs, 3 μm/yr [118 μin/yr] seems to be a bounding value under various geological repository environmental conditions. Mostly the data are distributed at the lower side (McCright, et al., 1987; Glass, et al., 1984; BSC, 2004b). A distribution type skewing toward lower end is reasonable.
SS_GC_Ox_Low	Stainless steel, low bound for the corrosion rate, oxidizing medium (μm/yr)	Constant 0.01	Based on Kursten, et al. (2004b, Table 4-34). This low rate is also near the resolution limit of the weight loss analysis method to determine corrosion rate.
SS_Prob_LC_Period_I _Oxidizing	Fraction of SS waste packages failed by LC during the early Period I in oxidizing environment (unitless)	Triangular 0.25, 0.45, 0.5	Probability of localized corrosion, per waste package, during Period I (see parameter LC_FailureTime_Period_I for Period I definition) in a repository in oxidizing media. Stainless steel has a greater chance of exhibiting localized corrosion in an oxidizing repository (oxidizing conditions prevail in the short and long terms). Based on the arguments for parameter SS_Prob_LC_Period_I_Reducing, 50 percent probability for LC is a reasonable number. Triangular distribution with apex at 0.45, mean at 0.4, median at 0.4.

Table A–2. Default Parameters for SOAR Waste Package Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
SS_Prob_LC_Period_I_Reducing	Fraction of SS waste packages failed by LC during the early Period I in reducing environment (unitless)	Triangular 0, 0.125, 0.25	Probability of localized corrosion, per waste package, during Period I (see parameter LC_FailureTime_Period_I for Period I definition) in a repository in reducing media. In this case, Period I is the transient oxidizing period prior to stable reducing period. 50 percent chance is a reasonable number, based on water compositions and 1,000 ppm chloride concentration for localized corrosion to occur. The backfill diffusive barrier could limit the chloride concentration in contact with stainless steel (assumed 50 percent chance for backfill to limit water contact). Max probability = 0.25 (0.5 × 0.5). A triangular distribution is used to determine the most likely value in the middle.
SS_Prob_LC_Period_II_Oxidizing	Fraction of SS waste packages failed by LC during the late Period II in oxidizing environment (unitless)	Constant 0	Probability of localized corrosion, per waste package, during Period II (see parameter LC_FailureTime_Period_II for Period II definition) in a repository in oxidizing media. It is assumed that all of the LC damage occurred during Period I; thus, this parameter is assigned a value of 0.
SS_Prob_LC_Period_II_Reducing	Fraction of SS waste packages failed by LC during the late Period II in reducing environment (unitless)	Uniform 0.01, 0.1	Probability of localized corrosion, per waste package, during Period II (see parameter LC_FailureTime_Period_II for Period II definition) in a repository in reducing media. Localized corrosion for reducing environments is less likely; backfill may be less effective to protect against localized corrosion. Assumed 5 percent average probability with a uniform distribution.

Table A–2. Default Parameters for SOAR Waste Package Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Ti_GC_Anox_High	Titanium, high bound for the corrosion rate, reducing medium (μm/yr)	Constant 0.2	The general corrosion rates are based on literature review of corrosion rates in possible repository conditions from international countries that proposed to use this material for nuclear waste disposal. Germany proposed to use Ti99.8-Pd, which is similar to Titanium Grade 7, as the container material under rock-salt condition. The corrosion rates from rock-salt brine were higher compared to those obtained from other media because of the more aggressive nature of the rock-salt brine. The corrosion rates from YMP titanium drip shield are considered to be appropriate because they cover a wide range of environmental conditions and experimental uncertainty (SNL, 2008). Other data reported are very close to this range (Brossia, et al., 2001; BSC, 2004; Blackwood, et al., 1988; Hua and Gordon, 2004; Schutz, 2005, 2003; Nakayama, et al., 2008). Data in oxidating and reducing conditions are similar.
Ti_GC_Anox_Low	Titanium, low bound for the corrosion rate, reducing medium (μm/yr)	Constant 0.008	The general corrosion rates are based on literature review of corrosion rates in possible repository conditions from international countries that proposed to use this material for nuclear waste disposal. Germany proposed to use Ti99.8-Pd, which is similar to Titanium Grade 7, as the container material under rock-salt condition. The corrosion rates from rock-salt brine were higher compared to those obtained from other media because of the more aggressive nature of the rock-salt brine. The corrosion rates from YMP titanium drip shield are considered to be appropriate because they cover a wide range of environmental conditions and experimental uncertainty (SNL, 2008). Other data reported are very close to this range (Brossia, et al., 2001; BSC, 2004; Blackwood, et al., 1988; Hua and Gordon, 2004; Schutz, 2005, 2003; Nakayama, et al., 2008). Data in oxidizing and reducing conditions are similar.

Table A–2. Default Parameters for SOAR Waste Package Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Ti_GC_Ox_High	Titanium, high bound for the corrosion rate, oxidizing medium (μm/yr)	Constant 0.2	The general corrosion rates are based on literature review of corrosion rates in possible repository conditions from international countries that proposed to use this material for nuclear waste disposal. Germany proposed to use Ti99.8-Pd, which is similar to Titanium Grade 7, as the container material under rock-salt condition. The corrosion rates from rock-salt brine were higher compared to those obtained from other media because of the more aggressive nature of the rock-salt brine. The corrosion rates from YMP titanium drip shield are considered to be appropriate because they cover a wide range of environmental conditions and experimental uncertainty (SNL, 2008). Other data reported are very close to this range (Brossia, et al., 2001; BSC, 2004; Blackwood, et al., 1988; Hua and Gordon, 2004; Schutz, 2005, 2003; Nakayama, et al., 2008). Data in oxidizing and reducing conditions are similar.
Ti_GC_Ox_Low	Titanium, low bound for the corrosion rate, oxidizing medium (μm/yr)	Constant 0.008	The general corrosion rates are based on literature review of corrosion rates in possible repository conditions from international countries that proposed to use this material for nuclear waste disposal. Germany proposed to use Ti99.8-Pd, which is similar to Titanium Grade 7, as the container material under rock-salt condition. The corrosion rates from rock-salt brine were higher compared to those obtained from other media because of the more aggressive nature of the rock-salt brine. The corrosion rates from YMP titanium drip shield are considered to be appropriate because they cover a wide range of environmental conditions and experimental uncertainty (SNL, 2008). Other data reported are very close to this range (Brossia, et al., 2001; Bechtel SAIC Company, LLC, 2004; Blackwood, et al., 1988; Hua and Gordon, 2004; Schutz, 2005, 2003; Nakayama, et al., 2008). Data in oxidizing and reducing conditions are similar.
WP_Thickness_CS	Carbon steel WP Thickness (cm)	Constant 10	International countries reported 3–25 cm [1.2–9.8 in] as the carbon steel container thickness. The rounded average value of 10 cm [3.9 in] is chosen.

Table A–2. Default Parameters for SOAR Waste Package Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
WP_Thickness_Cu	Copper WP Thickness (cm)	Constant 2.5	Canada proposes 2.5 cm [1 in] and both Finland and Sweden proposes 5 cm [2 in], based on Kursten, et al. (2004b, Table 1-1). The thinnest value of 2.5 cm [1 in] was chosen as the container thickness.
WP_Thickness_SS	Stainless steel WP Thickness (cm)	Constant 5	Based on YM inner container, not data available from other countries.
WP_Thickness_Ti	Titanium WP Thickness (cm)	Constant 1	Based on data from international countries: Canada proposes 6.35 mm [0.25 in]; Germany proposes 3–4 mm [0.12–0.16 in]; YM drip shield thickness is 15 mm [0.59 in]; no thickness data are available from Japan, although Kursten, et al. (2004b, Table 1-1) proposes Ti. Select 10 mm [0.39 in] as the thickness, which is near the average of all available data.

Table A–3. Default Parameters for SOAR Near Field Model Component			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Backfill_Porosity	Initial porosity of the backfill unit (unitless)	Constant 0.44	SKB (2006, Table A–8). Treated as constant for this model because variability is small compared to uncertainty in K_d values.
Backfill_SpecificDensity	Backfill specific density (kg/m^3)	Constant 2000	SKB (2006, Table A–8). Treated as constant for this model because variability is small compared to uncertainty in K_d values.
BF_dispersivityFraction	Dispersivity fraction of a backfill unit after cracking (unitless)	Uniform 0.05, 0.15	Typical range
BFtoFrac_dispersivity Fraction	Dispersivity fraction of transition region (unitless)	Uniform 0.1, 0.2	Typical range

Table A–3. Default Parameters for SOAR Near Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Dc_C_Backfill	Diffusivity of C in backfill material (m^2/s)	Uniform 3.0E-12, 3.0E-11	SKB (2006, Table A–11). Uniform distribution selected to equally weight full range of uncertainty. Note that range of values for diffusivity is smaller because carbonate species and organic acids are subject to anion exclusion.
Dc_C_Free	Diffusivity of C in free water (m^2/s)	Constant 1.20E-09	SKB (2006, Table A–40). Recommended diffusion coefficients in free solution are on the order of 1E-9 m^2/s, consistent with diffusion coefficients of electrolytes and nonelectrolytes in Weast (1986) at 25 °C [77 °F].
Dc_Cs_Backfill	Diffusivity of Cs in backfill material (m^2/s)	Uniform 4.94E-11, 1.91E-10	SKB (2006, Table A–11). Uniform distribution selected to equally weight full range of uncertainty.
Dc_Cs_Free	Diffusivity of Cs in free water (m^2/s)	Constant 2.10E-09	SKB (2006, Table A–40). Recommended value for diffusivities in free solution. The recommended diffusion coefficients in free solution are on the order of 1E-9 m^2/s, which are consistent with diffusion coefficients of electrolytes and nonelectrolytes in Weast (1986) at 25 °C [77 °F].
Dc_I_Backfill	Diffusivity of I in backfill material (m^2/s)	Uniform 3.0E-12, 3.0E-11	SKB (2006, Table A–11). Uniform distribution selected to equally weight full range of uncertainty. Note that range of values for Iodide is smaller because it is subject to anion exclusion.
Dc_I_Free	Diffusivity of I in free water (m^2/s)	Constant 8.30E-10	SKB (2006, Table A–40). Recommended value for diffusivities in free solution. The recommended diffusion coefficients in free solution are on the order of 1E-9 m^2/s, which are consistent with diffusion coefficients of electrolytes and nonelectrolytes in Weast (1986) at 25 °C [77 °F].

Table A–3. Default Parameters for SOAR Near Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Dc_Np_Backfill	Diffusivity of Np in backfill material (m^2/s)	Uniform 4.94E-11, 1.91E-10	SKB (2006, Table A–11). Uniform distribution selected to equally weight full range of uncertainty.
Dc_Np_Free	Diffusivity of Np in free water (m^2/s)	Constant 1.00E-09	SKB (2006, Table A–40). Recommended value for diffusivities in free solution. The recommended diffusion coefficients in free solution are on the order of 1E-9 m^2/s, which are consistent with diffusion coefficients of electrolytes and nonelectrolytes in Weast (1986) at 25 °C [77 °F].
Dc_Pu_Backfill	Diffusivity of Pu in backfill material (m^2/s)	Uniform 4.94E-11, 1.91E-10	SKB (2006, Table A–11). Uniform distribution selected to equally weight full range of uncertainty.
Dc_Pu_Free	Diffusivity of Pu in free water (m^2/s)	Constant 1.00E-09	(SKB, 2006). Table A–40. Recommended value for diffusivities in free solution. The recommended diffusion coefficients in free solution are on the order of 1E-9 m^2/s, which are consistent with diffusion coefficients of electrolytes and nonelectrolytes in Weast (1986) at 25 °C [77 °F].
Dc_Se_Backfill	Diffusivity of Se in backfill material. (m^2/s)	Uniform 3E-12, 3E-11	SKB (2006, Table A–11). Uniform distribution selected to equally weight full range of uncertainty.
Dc_Se_Free	Diffusivity of Se in free water (m^2/s)	Constant 2.10E-09	SKB (2006, Table A–40). Recommended value for diffusivities in free solution. The recommended diffusion coefficients in free solution are on the order of 1E-9 m^2/s, which are consistent with diffusion coefficients of electrolytes and nonelectrolytes in Weast (1986) at 25 °C [77 °F].

Table A–3. Default Parameters for SOAR Near Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Dc_Tc_Backfill	Diffusivity of Tc in backfill material (m^2/s)	Uniform 4.94E-11, 1.91E-10	SKB (2006, Table A–11). Uniform distribution selected to equally weight full range of uncertainty.
Dc_Tc_Free	Diffusivity of Tc in free water (m^2/s)	Constant 1.00E-09	SKB (2006, Table A–40). Recommended value for diffusivities in free solution. The recommended diffusion coefficients in free solution are on the order of 1E-9 m^2/s, which are consistent with diffusion coefficients of electrolytes and nonelectrolytes in Weast (1986) at 25 °C [77 °F].
Dc_U_Backfill	Diffusivity of U in backfill material (m^2/s)	Uniform 4.94E-11, 1.91E-10	SKB (2006, Table A–11). Uniform distribution selected to equally weight full range of uncertainty.
Dc_U_Free	Diffusivity of U in free water (m^2/s)	Constant 1.00E-09	SKB (2006, Table A–40). Recommended value for diffusivities in free solution. The recommended diffusion coefficients in free solution are on the order of 1E-9 m^2/s, which are consistent with diffusion coefficients of electrolytes and nonelectrolytes in Weast (1986) at 25 °C [77 °F].
f_DiffLengthToFracture	Fraction to compute the effective diffusive distance to the nearest fracture (unitless)	Uniform 0.1, 0.2	Stothoff (2010)
Kd_C_BF_Anox	K_d of C in backfill material, reducing conditions (m^3/kg)	Constant 0	SKB (2006, Table A–12) gives zero value for nonsorbing carbon.
Kd_C_BF_Ox	K_d of C in backfill material, oxidizing conditions (m^3/kg)	Constant 0	SKB (2006, Table A–12) gives zero value for nonsorbing carbon.

Table A–3. Default Parameters for SOAR Near Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Kd_Cs_BF_Anox	K_d of Cs in backfill material, reducing conditions (m^3/kg)	Log-uniform 0.018, 0.6	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended.
Kd_Cs_BF_Ox	K_d of Cs in backfill material, oxidizing conditions (m^3/kg)	Log-uniform 0.018, 0.6	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended.
Kd_I_BF_Anox	K_d of I in backfill material, reducing conditions (m^3/kg)	Constant 0	SKB (2006, Table A–12) gives zero value for nonsorbing iodine.
Kd_I_BF_Ox	K_d of I in backfill material, oxidizing conditions (m^3/kg)	Constant 0	SKB (2006, Table A–12) gives zero value for nonsorbing Iodine.
Kd_Np_BF_Anox	K_d of Np in backfill material, reducing conditions (m^3/kg)	Log-uniform 4, 1113	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended. For reducing conditions, Np(IV) is assumed.
Kd_Np_BF_Ox	K_d of Np in backfill material, oxidizing conditions (m^3/kg)	Log-uniform 0.004, 0.2	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended. For oxidizing conditions, Np(V) is assumed.
Kd_Pu_BF_Anox	K_d of Pu in backfill material, reducing conditions (m^3/kg)	Log-uniform 4, 1111	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended. For reducing conditions, range for both Pu(III) and Pu(IV) are included.
Kd_Pu_BF_Ox	K_d of Pu in backfill material, oxidizing conditions (m^3/kg)	Log-uniform 0.002, 28	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended. For oxidizing conditions, range for both Pu(V) and Pu(VI) are included.
Kd_Se_BF_Anox	K_d of Se in backfill material, reducing conditions (m^3/kg)	Log-uniform 0.003, 0.4	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended.

Table A–3. Default Parameters for SOAR Near Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Kd_Se_BF_Ox	K_d of Se in backfill material, oxidizing conditions (m^3/kg)	Constant 0	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended.
Kd_Tc_BF_Anox	K_d of Tc in backfill material, reducing conditions (m^3/kg)	Log-uniform 2.3, 1764	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended. For reducing conditions, Tc(IV) is assumed.
Kd_Tc_BF_Ox	K_d of Tc in backfill material, oxidizing conditions (m^3/kg)	Constant 0	SKB (2006, Table A–12) gives zero value for Tc(VII), which is assumed for oxidizing conditions.
Kd_U_BF_Anox	K_d of U in backfill material, reducing conditions (m^3/kg)	Log-uniform 3.6, 1113	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended. For reducing conditions, range for U(IV) is assumed.
Kd_U_BF_Ox	K_d of U in backfill material, oxidizing conditions (m^3/kg)	Log-uniform 0.5, 18	SKB (2006, Table A–12) provides range of minimum to maximum recommended values for bentonite buffer. Log-uniform distribution is also recommended. For oxidizing conditions, range for U(VI) is assumed.
Solubility_C_Ox	C solubility in backfill, oxidizing conditions (mg/L)	Log-uniform 8, 8.50E+02	SKB (2006, Table 8-1). Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm, indicating a value of 7.1E-3 mol/L for $CaCO^3$ as dominant carbonate species. This translates to a value of 85 mg/L. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below this value.
Solubility_C_Red	C solubility in backfill, reducing conditions (mg/L)	Log-uniform 4.8, 4.80E+02	SKB (2006, Table 8-1). Value for reducing conditions is based on the table column for bentonite, indicating a value of 3.99E-3 mol/L for $CaCO^3$ as dominant carbonate species. This translates to a value of 48 mg/L. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below this value.
Solubility_Cs_Ox	Cs solubility in backfill, oxidizing conditions (mg/L)	Constant -1	SKB (2006, Table 8-1). Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm. For Cs, this table indicates no solubility limit. The entered value of -1 tells the GoldSim model that this is the case.

Table A–3. Default Parameters for SOAR Near Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Solubility_Cs_Red	Cs solubility in backfill, reducing conditions (mg/L)	Constant -1	SKB (2006, Table 8-1). Value for reducing conditions is based on the table column for bentonite. For Cs, this table indicates no solubility limit. The entered value of -1 tells the GoldSim model that this is the case.
Solubility_I_Ox	I solubility in backfill, oxidizing conditions (mg/L)	Constant -1	No reference available for iodide solubility in oxidizing waters. Based on SKB (2006), indicates no solubility limit for Cs and Tc; it seems reasonable to assume the same for iodide.
Solubility_I_Red	I solubility in backfill, reducing conditions (mg/L)	Constant -1	No reference available for iodide solubility. Basecase assumes no solubility limit.
Solubility_Np_Ox	Np solubility in backfill, oxidizing conditions (mg/L)	Log-uniform 8.00E-01, 8.00E+01	SKB (2006, Table 8-1). Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm, indicating 1.7E-5 mol/L Np_2O_5, which translates to 8 mg/L. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below.
Solubility_Np_Red	Np solubility in backfill, reducing conditions (mg/L)	Log-uniform 2.6E-05, 2.6E-03	SKB (2006, Table 8-1). Value for reducing conditions is based on the table column for bentonite, indicating 1.1E-9 mol/L NpO_2, which translates to 2.6E-4 mg/L. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below.
Solubility_Pu_Ox	Pu solubility in backfill, oxidizing conditions (mg/L)	Log-uniform 5.4, 5.40E+02	SKB (2006, Table 8-1). Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm, indicating 2.2E-4 mo/L for $Pu(OH)_4$. This translates to 54 mg/L. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below this value.
Solubility_Pu_Red	Pu solubility in backfill, reducing conditions (mg/L)	Log-uniform 3.0E-01, 3.0E+01	SKB (2006, Table 8-1). Value for reducing conditions is based on the table column for bentonite, indicating 1.3E-5 mo/L of dominant phase $PuOHCO_3$. This translates to about 3 mg/L. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below this value.

Table A–3. Default Parameters for SOAR Near Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Solubility_Se_Ox	Se solubility in backfill, oxidizing conditions (mg/L)	Constant -1	SKB (2006, Table 8-1). Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm. For Cs, this table indicates no solubility limit. The entered value of -1 tells the GoldSim model that this is the case.
Solubility_Se_Red	Se solubility in backfill, reducing conditions (mg/L)	Constant -1	SKB (2006, Table 8-1). Value for reducing conditions is based on the table column for bentonite. For Cs, this table indicates no solubility limit. The entered value of -1 tells the GoldSim model that this is the case.
Solubility_Sn_Ox	Sn solubility in backfill, oxidizing conditions (mg/L)	Constant 8.60E-08	SKB (2006, Table 8-1). Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm.
Solubility_Sn_Red	Sn solubility in backfill, reducing conditions (mg/L)	Constant 8.60E-08	SKB (2006, Table 8-1). Value for reducing conditions is based on the table column for bentonite.
Solubility_Tc_Ox	Tc solubility in backfill, oxidizing conditions (mg/L)	Constant -1	SKB (2006, Table 8-1). Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm.
Solubility_Tc_Red	Tc solubility in backfill, reducing conditions (mg/L)	Log-uniform 4.0E-05, 4.0E-03	SKB (2006, Table 8-1). Value for reducing conditions is based on the table column for bentonite, indicating 4.4E-9 mo/L of dominant phase TcO_2. This translates to about 4E-4 mg/L. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below this value.
Solubility_U_Ox	U solubility in backfill, oxidizing conditions (mg/L)	Log-uniform 4.50E-01, 4.50E+01	SKB (2006, Table 8-1). Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm, which indicates 1.7 E-6 mol/L as uranophane plus 2.5E-6 mo/L as becquerelite. This translates to about 4.5 mg/L total uranium. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below this value.
Solubility_U_Red	U solubility in backfill, reducing conditions (mg/L)	Log-uniform 3.00E-01, 3.00E+01	SKB (2006, Table 8-1). Value for reducing conditions is based on the table column for bentonite, indicating 1.4E-5 mo/L of dominant phase uranophane. This translates to about 3 mg/L. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below this value.

Table A–4. Default Parameters for SOAR Far Field Model Component			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Density_Fractured	Bulk density of fractured rocks (kg/m^3)	Uniform 2000, 2500	SKB (2006, p. 125) suggests a generic value of 2,600 kg/m^3 [162 lb/ft^3] is appropriate for modeling because natural variability is not significant.
Density_Porous	Density of porous media (kg/m^3)	Uniform 2,100; 2,900	
Density_Sediments	Bulk Density of Sediments (kg/m^3)	Uniform 1,750; 2,070	DOE (2008, Table 6.3.10-2). Bulk density of alluvium mean value is 1,910 kg/m^2 with standard deviation of 78. Range given approximates mean plus or minus two standard deviations.
FF_DispersivityFraction	Dispersivity expressed as a fraction of the length of the FF transport pathway (unitless)	Constant 0.1	Base case will assume dispersion length is 10 percent of path length.
FF_L1_Fracture_Aperture	Effective aperture of fractures in leg 1 (m)	Log-uniform 1.00E-06, 1.00E-02	Effective fracture apertures are difficult to characterize and, therefore, highly uncertain. For base case we assume log-uniform distribution for a median value of 0.1 mm (10^{-4} m) [0.039 in] with two orders of magnitude uncertainty on either side.
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
FF_L1_Fracture_Separation	Distance between fractures with advective flow (m)	Log-uniform 5, 500	SKB (2006, Tables 6-42 and 6-3) provide average flowing interval frequencies for several granite borehole logs. Results indicate mean fracture spacings as low as 3 m [9.8 ft] to as high as 600 m [1,968 ft], but most average spacings on the order of several tens of meters. Log-uniform distribution from 5 to 500 m [16 to 1,640 ft] provides a reasonable approximation of these results with median value of 50 m [164 ft].

Table A–4. Default Parameters for SOAR Far Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
FF_L1_Hydraulic_K_PM	Hydraulic conductivity for porous rocks/soils (e.g., clay, siltstone) of leg 1 (m/s)	Log-triangular 1.00E-14, 1.00E-09, 1.00E-06	NEA (2005)
FF_L1_Hydraulic_K_Sed	Hydraulic conductivity for sedimentary rocks/soils of leg 1 (m/yr)	Log-uniform 5,500	DOE (2007, Table 7-4) indicates K_{sat} for combined test intervals in Well EWDP-19D were 55 m/yr [0.5 ft/d]. DOE (2007, Figure 7-4) plots results of other tests in alluvium and indicates uncertainty within an order of magnitude above and below this value. Log-uniform distribution selected to give median of 50 m/yr [164 ft/yr] and equal weight to each order of magnitude.
FF_L1_Matrix_Perimeter_f	Matrix Perimeter Fraction of Leg 1, used to define active perimeter for transversal mass exchange with the matrix (unitless)	Uniform 0.1, 1	Uniform distribution from 0.1 to 1.0 accounts for potential for most flow to be channeled within as little as 10 percent of the fracture volume.
FF_L2_Fracture_Aperture	Fracture Aperture of FF Leg 2 (m)	Log-uniform 1.00E-06, 1.00E-02	Effective fracture apertures are difficult to characterize and, therefore, highly uncertain. For base case we assume log-uniform distribution for a median value of 0.1 mm (10^{-4} m) [0.039 in] with two orders of magnitude uncertainty on either side.
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
FF_L2_Fracture_Separation	Distance between major fractures with advective flow (m)	Log-uniform 5, 500	SKB (2006, Tables 6-42 and 6-3) provide average flowing interval frequencies for several granite borehole logs. Results indicate mean fracture spacings as low as 3 m [9.84 ft] to as high as 600 m [1,968 ft], but most average spacings on the order of several tens of meters. Log-uniform distribution from 5 to 500 m [16 to 1,640 ft] provides a reasonable approximation of these results with median value of 50 m [164 ft].

Table A–4. Default Parameters for SOAR Far Field Model Component (continued)

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
FF_L2_Hydraulic_K_PM	Hydraulic conductivity for porous rocks/soils (e.g., clay, siltstone) of leg 2 (m/s)	Log-triangular 1.00E-14, 1.00E-09, 1.00E-06	NEA (2005)
FF_L2_Hydraulic_K_Sed	Hydraulic conductivity for sedimentary rocks/soils of leg 2 (m/yr)	Log-uniform 5,500	DOE (2007, Table 7-4) indicates K_{sat} for combined test intervals in Well EWDP-19D were 55 m/yr [0.5 ft/d]. DOE (2007, Figure 7-4) plots results of other tests in alluvium and indicates uncertainty within an order of magnitude above and below this value. Log-uniform distribution selected to give median of 50 m/yr [164 ft/yr] and equal weight to each order of magnitude.
FF_L2_Matrix_Perimeter_f	Matrix Perimeter Fraction of FF leg 2 (unitless)	Uniform 0.1, 1	Uniform distribution from 0.1 to 1.0 accounts for potential for most flow to be channeled within as little as 10 percent of the fracture volume.
FF_L3_Fracture_Aperture	Fracture Aperture of FF leg 3 (m)	Log-uniform 1.00E-06, 1.00E-02	Effective fracture apertures are difficult to characterize and, therefore, highly uncertain. For base case we assume log-uniform distribution for a median value of 0.1 mm (1E-4 m) [0.039 in] with two orders of magnitude uncertainty on either side.
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
FF_L3_Fracture_Separation	Distance between major fractures with advective flow (m)	Log-uniform 5, 500	SKB (2006, Tables 6-42 and 6-3) provide average flowing interval frequencies for several granite borehole logs. Results indicate mean fracture spacings as low as 3 m [9.8 ft] to as high as 600 m [1,968 ft], but most average spacings on the order of several tens of meters. Log-uniform distribution from 5 to 500 m [16.4 to 1,640 ft] provides a reasonable approximation of these results with median value of 50 m [164 ft].
FF_L3_Hydraulic_K_PM	Hydraulic conductivity for porous rocks/soils (clay, siltstone etc.) of leg 3 (m/s)	Log-triangular 1.00E-14, 1.00E-09, 1.00E-06	NEA (2005)

Table A–4. Default Parameters for SOAR Far Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
FF_L3_Matrix_Perimeter_f	Matrix Perimeter Fraction of FF leg 3 (unitless)	Uniform 0.1, 1	Uniform distribution from 0.1 to 1.0 accounts for potential for most flow to be channeled within as little as 10 percent of the fracture volume.
Kd_C_Fractured_Anox	K_d of C in fractured rock, reducing conditions (m^3/kg)	Constant 0	Treated as nonsorbing anion
Kd_C_Fractured_Ox	K_d of C in fractured rock, oxidizing conditions (m^3/kg)	Constant 0	Treated as nonsorbing anion
Kd_C_Porous_Anox	K_d of C in porous media, reducing conditions (m^3/kg)	Log-uniform 1.00E-04, 1	Nirex Limited United Kingdom (2003)
Kd_C_Porous_Ox	K_d of C in porous media, oxidizing conditions (m^3/kg)	Constant 0	Treated as nonsorbing anion
Kd_C_Sed_Anox	K_d of C in porous rock, reducing conditions (m^3/kg)	Uniform 0, 2.0	Brady, et al. (2009, Table 5)
Kd_C_Sed_Ox	K_d of C in porous rock, oxidizing conditions (m^3/kg)	Constant 0	DOE (2008, Table 6.3.10-1) identifies as nonsorbing
Kd_Cs_Fractured_Anox	K_d of Cs in fractured rock, reducing conditions (m^3/kg)	Log-uniform 4.00E-05, 2.00E-01	SKB (2006, Table A–43) range of high and low values for Cs(I) in saline waters multiplied by correction factor 0.1. Log-uniform distribution recommended by SKB panel.
Kd_Cs_Fractured_Ox	K_d of Cs in fractured rock, oxidizing conditions (m^3/kg)	Log-uniform 4.00E-05, 2.00E-01	SKB (2006, Table A–43) range of high and low values for Cs(I) in saline waters multiplied by correction factor 0.1. Log-uniform distribution recommended by SKB panel.
Kd_Cs_Porous_Anox	K_d of Cs in porous media, reducing conditions (m^3/kg)	Log-uniform 10, 290	SKB (1997)
Kd_Cs_Porous_Ox	K_d of Cs in porous media, oxidizing conditions (m^3/kg)	Log-uniform 10, 2.90E+02	SKB (1997)
Kd_Cs_Sed_Anox	K_d of Cs in porous rock, reducing conditions (m^3/kg)	Log-uniform 100, 1000	DOE (2008, Table 6.3.10-2) provides minimum and maximum for range. Log-uniform gives equal weight to each order of magnitude of uncertainty range.
Kd_Cs_Sed_Ox	K_d of Cs in porous rock, oxidizing conditions (m^3/kg)	Log-uniform 100, 1000	DOE (2008, Table 6.3.10-2) provides minimum and maximum for range. Log-uniform gives equal weight to each order of magnitude of uncertainty range.

Table A–4. Default Parameters for SOAR Far Field Model Component (continued)			
Parameter Name	Description	Distribution Type & Values	Reference/Rationale
Kd_I_Fractured_Anox	K_d of I in fractured rock, reducing conditions (m^3/kg)	Constant 0	Treated as a nonsorbing anion
Kd_I_Fractured_Ox	K_d of I in fractured rock, oxidizing conditions (m^3/kg)	Constant 0	Treated as nonsorbing anion
Kd_I_Porous_Anox	K_d of I in porous media, reducing conditions (m^3/kg)	Log-uniform 0.001, 0.01	SKB (1997)
Kd_I_Porous_Ox	K_d of I in porous media, oxidizing conditions (m^3/kg)	Constant 0	Treated as nonsorbing anion
Kd_I_Sed_Anox	K_d of I in porous rock, reducing conditions (m^3/kg)	Uniform 0, 0.1	Brady, et al. (2009, Table 5)
Kd_I_Sed_Ox	K_d of I in porous rock, oxidizing conditions (m^3/kg)	Constant 0	DOE (2008, Table 6.3.10-1) identifies iodine as nonsorbing.
Kd_I_Porous_Anox	K_d of I in porous media, reducing conditions (m^3/kg)	Log-uniform 0.001, 0.01	SKB (1997)
Kd_I_Porous_Ox	K_d of I in porous media, oxidizing conditions (m^3/kg)	Constant 0	Treated as nonsorbing anion
Kd_I_Sed_Anox	K_d of I in porous rock, reducing conditions (m^3/kg)	Uniform 0, 0.1	Brady, et al. (2009, Table 5)
Kd_I_Sed_Ox	K_d of I in porous rock, oxidizing conditions (m^3/kg)	Constant 0	DOE (2008, Table 6.3.10-1) identifies iodine as nonsorbing.
Kd_Np_Fractured_Anox	K_d of Np in fractured rock, reducing conditions (m^3/kg)	Log-uniform 4.70E-03, 2	SKB (2006, Table A–43) range of high and low values for Np(IV) in saline waters multiplied by correction factor 0.1. Log-uniform distribution recommended by SKB panel.
Kd_Np_Fractured_Ox	K_d of Np in fractured rock, oxidizing conditions (m^3/kg)	Log-uniform 2.00E-04, 2.20E-02	SKB (2006, Table A–43) range of high and low values for Np(V) in saline waters multiplied by correction factor 0.1. Log-uniform distribution recommended by SKB panel.
Kd_Np_Porous_Anox	K_d of Np in porous media, reducing conditions (m^3/kg)	Log-uniform 1.00E-02, 5.00E+01	Nirex Limited United Kingdom (2003)
Kd_Np_Porous_Ox	K_d of Np in porous media, oxidizing conditions (m^3/kg)	Log-uniform 1.00E-04, 5.00E+00	Nirex Limited United Kingdom (2003)

Table A–4. Default Parameters for SOAR Far Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Kd_Np_Sed_Anox	K_d of Np in porous rock, reducing conditions (m^3/kg)	Log-uniform 1.8, 13	DOE (2008, Table 6.3.10-2) provides minimum and maximum for range. Log-uniform distribution gives equal weight to each order of magnitude of uncertainty range.
Kd_Np_Sed_Ox	K_d of Np in porous rock, oxidizing conditions (m^3/kg)	Log-uniform 1.8, 13	DOE (2008, Table 6.3.10-2). Reference provides minimum and maximum for range. Log-uniform distribution gives equal weight to each order of magnitude of uncertainty range.
Kd_Pu_Fractured_Anox	K_d of Pu in fractured rock, reducing conditions (m^3/kg)	Log-uniform 0.1, 1	SKB (2006, Table A–44) range of high and low values for Pu(III, IV) in saline waters multiplied by correction factor 0.1. Log-uniform distribution recommended by SKB panel.
Kd_Pu_Fractured_Ox	K_d of Pu in fractured rock, oxidizing conditions (m^3/kg)	Log-uniform 0.1, 1	SKB (2006, Table A–44) range of high and low values for Pu(III, IV) in saline waters multiplied by correction factor 0.1. Log-uniform distribution recommended by SKB panel.
Kd_Pu_Porous_Anox	K_d of Pu in porous media, reducing conditions (m^3/kg)	Log-uniform 1, 5.00E+03	Nirex Limited United Kingdom (2003)
Kd_Pu_Porous_Ox	K_d of Pu in porous media, oxidizing conditions (m^3/kg)	Log-uniform 74,999, 75,001	Mercer, et al. (1982)
Kd_Pu_Sed_Anox	K_d of Pu in porous rock, reducing conditions (m^3/kg)	Log-uniform 50, 300	DOE (2008, Table 6.3.10-2) provides minimum and maximum for range. Log-uniform distribution gives equal weight to each order of magnitude of uncertainty range.
Kd_Pu_Sed_Ox	K_d of Pu in porous rock, oxidizing conditions (m^3/kg)	Log-uniform 50, 300	DOE (2008, Table 6.3.10-2) provides minimum and maximum for range. Log-uniform distribution give equal weight to each order of magnitude of uncertainty range.
Kd_Se_Fractured_Anox	K_d of Se in fractured rock, reducing conditions (m^3/kg)	Constant 1.00E-03	SKB (1999, Table 2-13)
Kd_Se_Porous_Anox	K_d of Se in porous media, reducing conditions (m^3/kg)	Log-uniform 1.00E-06, 2	Nirex Limited United Kingdom (2003)
Kd_Se_Porous_Ox	K_d of Se in porous media, oxidizing conditions (m^3/kg)	Log-uniform 1.00E-06, 1	Nirex Limited United Kingdom (2003)

Table A–4. Default Parameters for SOAR Far Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Kd_Se_Sed_Anox	K_d of Se in porous rock, reducing conditions (m^3/kg)	Constant 0	DOE (2008, Table 6.3.10-1) identifies as nonsorbing
Kd_Se_Sed_Ox	K_d of Se in porous rock, oxidizing conditions (m^3/kg)	Constant 0	DOE (2008, Table 6.3.10-1) identifies as nonsorbing
Kd_Tc_Fractured_Anox	K_d of Tc in fractured rock, reducing conditions (m^3/kg)	Constant 0	Treated as nonsorbing anion
Kd_Tc_Fractured_Ox	K_d of Tc in fractured rock, oxidizing conditions (m^3/kg)	Constant 0	Treated as nonsorbing anion
Kd_Tc_Porous_Anox	K_d of Tc in porous media, reducing conditions (m^3/kg)	Log-uniform 1.00E-04, 250	Nirex Limited United Kingdom (2003) (Low), EPA (2004a) (High)
Kd_Tc_Porous_Ox	K_d of Tc in porous media, oxidizing conditions (m^3/kg)	Log-uniform 1.00E-06, 5.00E-01	Nirex Limited United Kingdom (2003)
Kd_Tc_Sed_Anox	K_d of Tc in porous rock, reducing conditions (m^3/kg)	Uniform 0, 1.0	Brady, et al. (2009, Table 5)
Kd_Tc_Sed_Ox	K_d of Tc in porous rock, oxidizing conditions (m^3/kg)	Constant 0	DOE (2008, Table 6.3.10-1) identifies as nonsorbing.
Kd_U_Fractured_Anox	K_d of U in fractured rock, reducing conditions (m^3/kg)	Log-uniform 4.80E-03, 2.80E-01	SKB (2006, Table A–43) range of high and low values for U(IV) in saline waters multiplied by correction factor 0.1. Log-uniform distribution recommended by SKB panel.
Kd_U_Fractured_Ox	K_d of U in fractured rock, oxidizing conditions (m^3/kg)	Log-uniform 5.00E-05, 1.20E-02	SKB (2006, Table A–43) range of high and low values for U(VI) in saline waters multiplied by correction factor 0.1. Log-uniform distribution recommended by SKB panel.
Kd_U_Porous_Anox	K_d of U in porous media, reducing conditions (m^3/kg)	Log-uniform 1, 5.00E+03	Nirex Limited United Kingdom (2003)
Kd_U_Sed_Anox	K_d of U in porous rock, reducing conditions (m^3/kg)	Log-uniform 1.7, 8.9	DOE (2008, Table 6.3.10-2) provides minimum and maximum for range. Log-uniform distribution gives equal weight to each order of magnitude of uncertainty range.

Table A–4. Default Parameters for SOAR Far Field Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Kd_U_Sed_Ox	K_d of U in porous rock, oxidizing conditions (m^3/kg)	Log-uniform 1.7, 8.9	DOE (2008, Table 6.3.10-2) provides minimum and maximum for range. Log-uniform distribution give equal weight to each order of magnitude of uncertainty range.
Porosity_Fractured	Porosity of Fractured Rocks—Use Granite (unitless)	Uniform 6.80E-04, 1.50E-03	(SKB, 2006). Table A-42 indicates log-10 mean porosity for three different granites ranging from -2.84 to -3.17.
Porosity_Porous	Porosity of porous media—use clay (unitless)	Uniform 0.05, 0.4	NEA (2005, Figure 23)
Porosity_Sediments	Porosity of Sediments (unitless)	Uniform 0.07, 0.3	DOE (2008, Table 6.3.10-2). Porosity of differentiated valley fill mean value of 0.18 with standard deviation of 0.051. Range given is mean ±2-sigma/

Table A–5. Default Parameters for SOAR Biosphere Model Component			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
Capture_Fraction	Capture_Fraction parameter modifies the concentration of radionuclides in water and accounts for the fraction of water accessible to the biosphere that is contaminated and/or fraction of total radionuclide mass from the far field that is transferred to the biosphere (unitless)	Constant 1	None. Initial value of unity does not change concentration calculation.
Ingestion_Dose_ Coefficient	Radiological dose to an adult from the ingestion of a unit activity of radionuclides in the vector (Sv/Bq) [C14, Cs135, I129, Np237, Pu238, Pu239, Pu240, Pu242, Se79, Tc99, U232, U233, U234, U235, U236, U238]	Constant-vector [5.80E-10, 2.00E-09, 1.10E-07, 1.10E-07, 2.30E-07, 2.50E-07, 2.50E-07, 2.40E-07, 6.40E-10, 3.30E-07, 5.10E-08, 4.90E-08, 4.70E-08, 4.70E-08, 4.50E-08]	ICRP (1996, Table A.1)

Table A–5. Default Parameters for SOAR Biosphere Model Component (continued)			
Parameter Name	**Description**	**Distribution Type & Values**	**Reference/Rationale**
WaterFlowToBiosphere	Water flow rate to the biosphere used to calculate radionuclide concentrations in water available at the interface between the far field and biosphere (ac-ft/yr)	Triangular 370, 1980, 5770	USDA (2008, Table 11)
Water_Consumption_Rate	Population-averaged consumption rate of well water for adults in the United States (L/yr)	Beta 380, 262, 24, 1023	EPA (2004b, Table A1, Appendix E, p. E–4)

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APPENDIX B
GLOSSARY

GLOSSARY

Abstraction: Reduction and representation of the essential and complex components of a feature, event, or process into a simplified form for inclusion in a model. An abstraction is intended to maximize the use of limited computational resources while allowing a sufficient range of sensitivity and uncertainty analyses.

Advection: The process in which solutes, particles, or molecules are transported by the motion of flowing fluid.

Ambient: Undisturbed, natural conditions.

Anoxic: Pertaining to the existence of reducing conditions; often due to minimal or no oxygen present.

Aqueous: Pertaining to water, such as aqueous phase, aqueous species, or aqueous transport.

Backfill: Materials used to fill in an excavated, open area after emplacement of waste.

Breach: A penetration in the waste package.

Center for Nuclear Waste Regulatory Analyses (CNWRA®): A federally funded research and development center in San Antonio, Texas, sponsored by the U.S. Nuclear Regulatory Commission (NRC), to provide NRC with technical assistance for the repository safety program.

Cladding: The metal outer sheath of a fuel rod generally made of a zirconium alloy intended to protect the uranium dioxide pellets, which are the nuclear fuel, from direct contact with reactor coolants or neutron moderators and dissolution by exposure to high temperature water under operating conditions in a reactor.

Colloid: As applied to radionuclide migration, a colloidal system is a group of large molecules or small particles having at least one dimension with the size range of 10^{-9} to 10^{-6} m [3.9×10^{-7} to 3.9×10^{-4} in] that are suspended in a solvent. Colloids that are transported in groundwater can be filtered out of the water in small pore spaces or very narrow fractures because of the large size of the colloids.

Conceptual Model: A set of descriptive features used to characterize a system or subsystem for a given purpose in a model. These features are compatible with one another and fit the existing data within the context of the given purpose of the model.

Corrosion: The deterioration of a material, usually a metal, as a result of a chemical or electrochemical reaction with its environment.

Criticality: The condition in which a fissile material sustains a chain reaction. It occurs when the number of neutrons present in one generation cycle equals the number generated in the previous cycle. The state is considered critical when a self-sustaining nuclear chain reaction is ongoing.

Diffusion: (i) The spreading or dissemination of a substance caused by concentration gradients. (ii) The gradual mixing of the molecules of two or more substances because of random thermal motion.

Diffusive Transport: Movement of solutes because of their concentration gradient. It is the process in which substances carried in groundwater move through the subsurface by means of diffusion because of a concentration gradient.

Dispersion: (i) The tendency of a solute (substance dissolved in groundwater) to spread out from the path it is expected to follow if only the bulk motion of the flowing fluid were to move it. (ii) The macroscopic outcome of the actual movement of individual solute particles through a porous medium. Dispersion causes dilution of solutes, including radionuclides, in ground water and is usually an important mechanism for spreading contaminants in low flow velocities.

Disruptive Event: An off-normal event that, in the case of the potential geologic disposal system, may include volcanic activity, seismic activity, and nuclear criticality. Disruptive events have two possible effects: (i) direct release of radioactivity to the surface or (ii) alteration of the nominal behavior of the system.

Dissolution: (i) Change from a solid to a liquid state. (ii) Dissolving a substance in a solvent.

Distribution: The overall scatter of values for a set of observed data. Distributions have structures that are the probability that a given value occurs in the set.

Drip Shield: A metallic structure placed along the extension of the emplacement area and above the waste packages to prevent seepage water from directly dripping onto the waste package outer surface.

Effective Porosity: The fraction of a porous medium volume available for fluid flow and/or solute transport, as in the saturated zone. Effective porosity is less than or equal to the total void space (porosity).

Equilibrium: The state of a chemical system in which the phases do not undergo any spontaneous change in properties or proportions with time; the system is under a dynamic balance in which the net rate of addition or depletion of masses or phases is zero.

Events: (i) Occurrences that have a specific starting time and, usually, a duration shorter than the time being simulated in a model. (ii) Uncertain occurrences that take place within a short time relative to the time frame of the model.

Features: Physical, chemical, thermal, or temporal components of a system or site.

Flow: The movement of a fluid such as air, water, or magma. Flow and transport are processes that can move radionuclides from a geologic disposal system to the biosphere.

Flow Pathway: The subsurface course that water or a solute (including radionuclides) would follow in a given groundwater velocity field, governed principally by the hydraulic gradient.

Fracture: A discontinuity in rock along which loss of cohesion has occurred. It is often caused by the stresses that cause folding and faulting. Fractures may act as fast paths for groundwater movement.

General Corrosion: A type of corrosion attack (deterioration) more or less uniformly distributed over a metal surface; corrosion that proceeds at approximately the same rate over a metal surface. Also called uniform corrosion.

Geochemical: Characterizing the distribution and amounts of the chemical elements in minerals, ores, rocks, soils, water, and the atmosphere; the movement of the elements in nature on the basis of their properties.

Geologic Disposal System: A set of integrated components within natural, geologic formations and with a function to isolate radioactive waste from the general population for a long period of time.

Groundwater: Water contained in pores or fractures in either the unsaturated or saturated zones below ground level.

High-Level Waste: A waste form produced by separating fissile material from fission products in spent nuclear fuel; the nonuseable material from current recycling technology.

Hydrologic: Pertaining to the properties, distribution, and circulation of water on the surface of the land, in the soil and underlying rocks, and in the atmosphere.

Isothermal: Having a constant temperature.

Localized Corrosion: Corrosion at discrete sites (e.g., pitting and crevice corrosion).

Matrix: Rock material and its pore space exclusive of fractures.

Matrix Diffusion: The process by which molecular or ionic solutes, such as radionuclides in ground water, move from areas of higher concentration to areas of lower concentration. This movement is through the pore spaces of the rock material as opposed to movement through the fractures.

Model: A depiction or representation of a system, phenomenon, or process, including any hypotheses required to describe the system or explain the phenomenon or process. Examples are conceptual, physical, mathematical, and numerical models.

Near Field: The area and conditions within a geologic disposal system including rock immediately surrounding the waste packages. The region within a geologic disposal system where the natural hydrogeologic system has been significantly impacted by the excavation of a geologic disposal system and the emplacement of waste.

U.S. Nuclear Regulatory Commission (NRC): An independent agency, established by the U.S. Congress under the Energy Reorganization Act of 1974, to ensure adequate protection of the public health and safety, the common defense and security, and the environment in the use of nuclear materials in the United States. Responsibility of NRC includes regulation of the transport, storage, and disposal of nuclear materials and waste.

Oxic: Pertaining to the existence of oxidizing conditions, due to the presence of oxygen.

Oxidation State: The chemical state of a radionuclide as a function of the number of electrons. The oxidation state is lower in anoxic (reducing) environments than in oxic (oxidizing) environments.

Parameter: Quantitative properties (e.g., data, values), together with principles or equations governing the behavior of a system, that are major constituents of computer codes for a mathematical or numerical model.

Pathway: A potential route by which radionuclides might reach the biosphere and pose a threat to humans. For example, direct exposure is an external pathway, and inhalation and ingestion are internal pathways.

Performance: A quantitative or qualitative result of the long-term evolution of a component, combination of components, or the whole geologic disposal system.

Permeability: The ability of a material to transmit fluid through its pores when subjected to a difference in pressure (pressure gradient).

Phase: A physically homogeneous and distinct portion of a material system, such as the gaseous, liquid, and solid phases of a substance.

Pitting Corrosion: Localized corrosion of a metal surface, confined to a small area, that takes the form of cavities named pits.

Porosity: The ratio of openings, or voids, to the total volume of a soil or rock expressed as a decimal fraction or as a percentage. See also *effective porosity*.

Probability: The chance that an outcome will occur from the set of possible outcomes. Statistical probability examines actual events and can be verified by observation or sampling. Knowledge of the exact probability of an event is usually limited by the inability to know, or compile, the complete set of possible outcomes over time or space.

Probability Distribution: The set of outcomes (values) and their corresponding probabilities for a random variable.

Processes: A series of actions that have gradual, continuous interactions with the system being modeled.

Radiolysis: Dissociation of molecules by the action of radiation.

Radionuclide: Radioactive type of atom with an unstable nucleus that spontaneously decays, usually emitting ionizing radiation in the process.

Receptor: An individual for whom radiological doses are calculated or measured.

Redox: Pertaining to the magnitude that a system is anoxic or oxic.

Retardation: Slowing radionuclide movement in ground water by mechanisms that include sorption of radionuclides, diffusion into rock matrix pores, and microfractures.

Risk: The probability that an undesirable event will occur, multiplied by the consequences of the undesirable event.

Rock Matrix: See *Matrix*.

Scenario: A well-defined, connected sequence of features, events, and processes that can be thought of as an outline of a possible future condition of a geologic disposal system. Scenarios can be undisturbed, in which case the performance would be the expected behavior for the system. Scenarios can also be disturbed, if altered by disruptive events.

Scoping Tool*:* A model specifically developed to gain preliminary risk and performance insights on a geologic disposal system.

Sorb: To undergo a process of sorption.

Sorption: The binding, on a microscopic scale, of one substance to another. A term that includes both adsorption and absorption. The sorption of dissolved radionuclides onto aquifer solids or waste package materials by means of close-range chemical or physical forces is potentially an important process in a geologic disposal system. Sorption is a function of the chemistry of the radioisotopes, the fluid in which they are carried, and the mineral material they encounter along the flow path.

***Sorption Coefficient* (K_d)**: Coefficient characterizing the affinity by which one substance binds to another.

Source Term: Types and amounts of radionuclides that are the source of a potential release. In the Scoping of Options and Analyzing Risk (SOAR), the source term included both the Waste Form Component and the Waste Package Component.

Spent Nuclear Fuel: Fuel that has been withdrawn from a nuclear reactor following irradiation, the constituent elements of which have not been separated by reprocessing. This fuel is more radioactive than it was before irradiation and releases significant amounts of heat from the decay of its fission product radionuclides.

Stress Corrosion Cracking: A cracking process that requires the simultaneous action of a corrosive material and sustained (residual or applied) tensile stress. Stress corrosion cracking excludes both the fracture of already corroded sections and the localized corrosion processes that can disintegrate an alloy without the action of residual or applied stress.

Transparency: The ease of understanding the process by which a study was carried out, which assumptions are driving the results, how they were arrived at, and the rigor of the analyses leading to the results. Transparency is achieved when a reader or reviewer has a clear picture of what was done in the analysis, what the outcome was, and why this outcome was produced.

Transport: A process that allows substances, such as contaminants or radionuclides, to be carried in a fluid through (i) the physical mechanisms of convection, diffusion, and dispersion and (ii) the chemical mechanisms of sorption, leaching, precipitation, dissolution, and complexation. Types of transport include advective, diffusive, and colloidal.

Uncertainty: How much a calculated or measured value varies from the unknown true value.

Variable: A nonunique property or attribute.

Variability: A measure of how a quantity varies over time or space.

APPENDIX C
LINKING A DATABASE TO A MODEL FILE

LINKING A DATABASE TO A MODEL FILE

Parameter values of the Scoping of Options and Analyzing Risk (SOAR) model are centrally managed with a Microsoft® Access® database. The following instructions describe the steps necessary to set up a connection between the SOAR model and a Microsoft Access database. There are four steps involved in linking a model element that defines a model parameter to a database. Administrator privilege may be necessary to execute some of the steps described next.

(1) Create a database that is compatible with GoldSim.

There are three types of Microsoft Access databases that can directly interface with GoldSim (see GoldSim Technology Group, LLC, 2010, Appendix F). The SOAR model uses the Yucca Mountain Database type. The database file *FPA-SOAR.mdb* has been prepared by the development team to be compatible with this type and is required for the proper operation of the SOAR model.

(2) Add the database as a *data source* to the host computer.

Administrator privilege may be required to connect an Access database to the host computer's Data Source Management. To make the Access database visible to GoldSim models

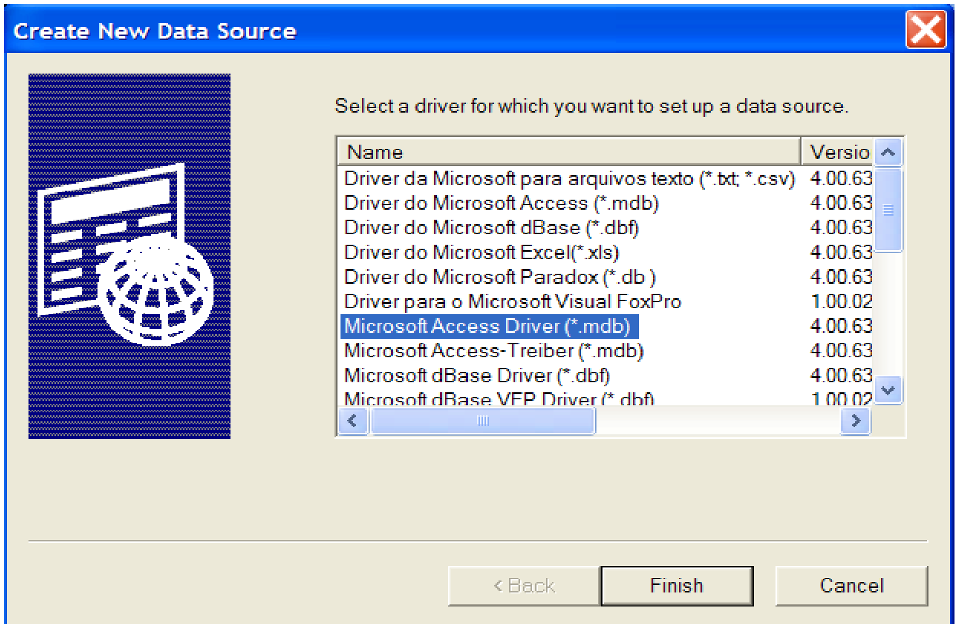
a. Open the Microsoft Windows® Control Panel (Start ⇒ Settings ⇒ Control Panel)

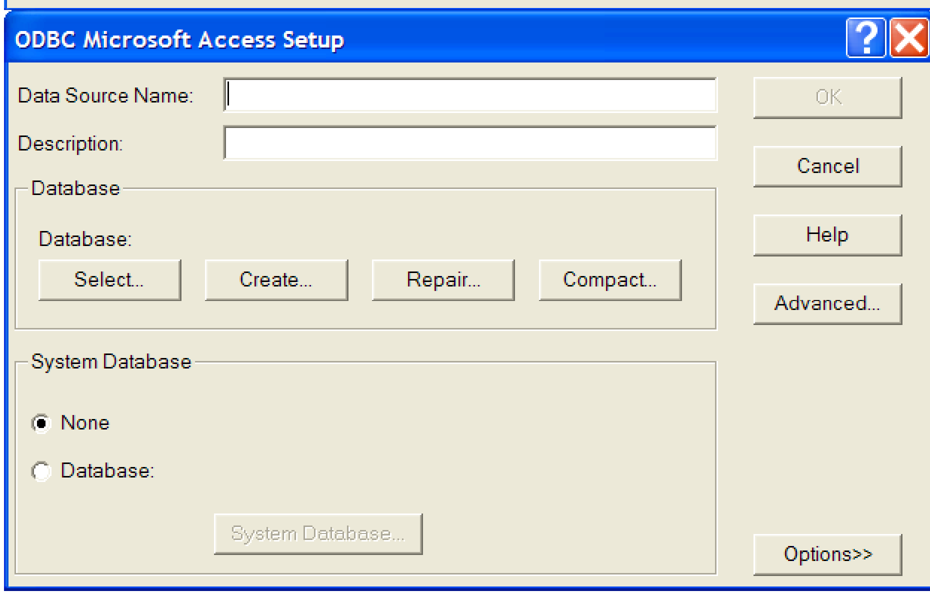
b. Open Administrative Tools

c. Open Data Sources (ODBC)

d. Click Add, which will open the following selection window

e. Select Microsoft Access Driver (*.mdb) and click Finish.

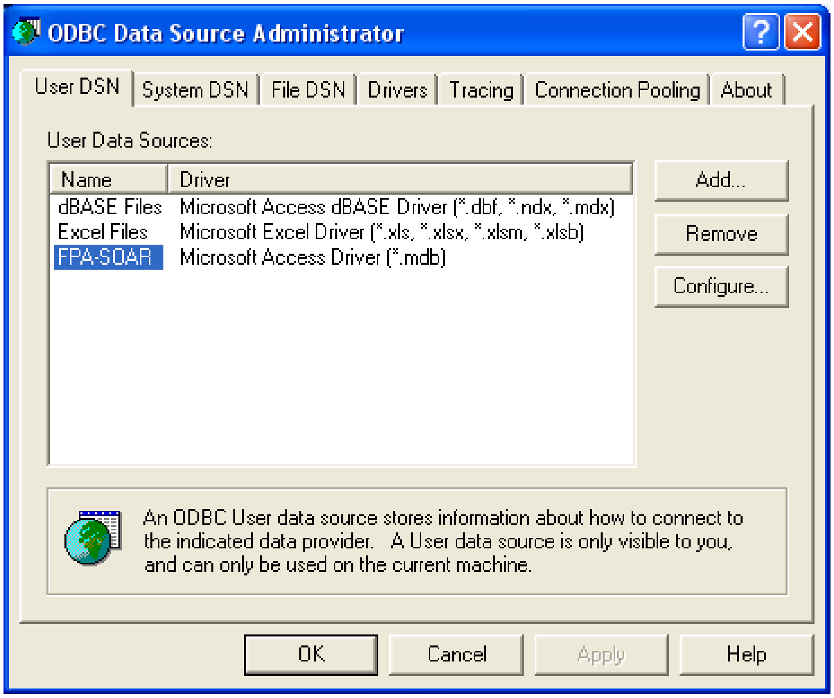




f. A setup dialog box will open up as follows.

g. The SOAR model requires that the Data Source Name be “FPA-SOAR.” Enter “FPA-SOAR” in the Data Source Name field, provide a description in the Description field, then click Select.

h. In the Select Database dialog box, locate and select the “Access Database” and click OK.



i. Click OK to close other dialog boxes. The Data Source Name from the ODBC Microsoft Access Setup window must appear in the ODBC Data Source Administration window under the User DSN tab for successful database updates to be performed.

(3) Link all elements in the model that use a centrally managed parameter to the database.

In the SOAR model the following elements can be downloaded from a database:

- Data elements (scalar, vector, and matrix)
- Lookup Table elements (1-D or 2-D tables)
- Stochastic elements

The SOAR model requires the element's Data Source property be set to "Yucca Mountain Database" on the Definition tab of the element's "Properties" window.

(4) Download the database information.

There are two ways that parameter values can be downloaded to the SOAR model:

- On the GoldSim shortcut menu bar, click on "DB" and select the data source. This downloads parameter values for all input elements in the model.

- Double-click an element; select the Database tab; in the Database field, select the data source; click "Download Now."

Reference

GoldSim Technology Group, LLC. "GoldSim User's Guide, Volume 2, Appendix F." Issaquah, Washington: GoldSim Technology Group, LLC. 2010.

APPENDIX D
SOAR EXAMPLE APPLICATION

SOAR Example Application

In this appendix, an example set of results is presented to show the types of analyses that can be performed with the intermediate and final results available in the SOAR model. This particular example shows the release and dose responses to changes in inputs controlled from the dashboard. Each run included 150 Monte Carlo realizations. The simulation is a family of runs with a single parameter (Degradation rate multiplier) varying discretely over a broad range. A summary report describes the objective of the simulation and the changed parameters, and it includes both release versus time plots and dose versus time plots. The waste package was assumed to fail instantaneously for all runs of the set. Release and dose data for Tc-99, I-129, and Np-237 are included to exhibit representative results for fission products and actinides. No interpretation of the results is provided. The plots summarize outputs from several runs, consolidated and plotted using Excel; i.e., the plots are not directly available on the SOAR results dashboard.

To define the Base Scenario, the SOAR Version 1.0.02 default settings were used except for the following Input Control changes.

- Run each simulation for 150 realizations, and save histories for 150 realizations.

- Set “Minimum waste package failure rate (waste packages per year)” equal to 0.999e6, “Maximum waste package failure rate (waste packages per year)” equal to 1e6, “End time of waste package failure (year)” equal to 1.01, and “Type of disruptive event” as “Waste package failure rate” to simulate instant waste package failure.

- Activate “Bypass the backfill (diffusive barrier).”

- Set all 2010 inventories equal to zero.

Simulation Summary Report

Objective: Show the effect on radionuclide release and dose of varying degradation rate for spent nuclear fuel in reducing environments.

Test Environment: GoldSim Player 10.5 SP1

SOAR Version: 1.0.02

Input Control Changes:

– Set “Additional Radionuclide Inventory (Total Waste Mass in Metric Tons)” for spent nuclear fuel equal to 100,000 MT.

– Set “degradation rate multiplier” equal to 1e+2, 1e+0, 1e-2, 1e-4, and 1e-6 in separate simulations.

– Set the Redox condition as “Reducing” for far-field legs one, two, and three.

Results: Simulations were performed, and results are provided on the following pages. Plots include time histories of waste form release, near field backfill release, far field leg 3 release, total dose, and individual dose for I-129, Tc-99, and Np-237.

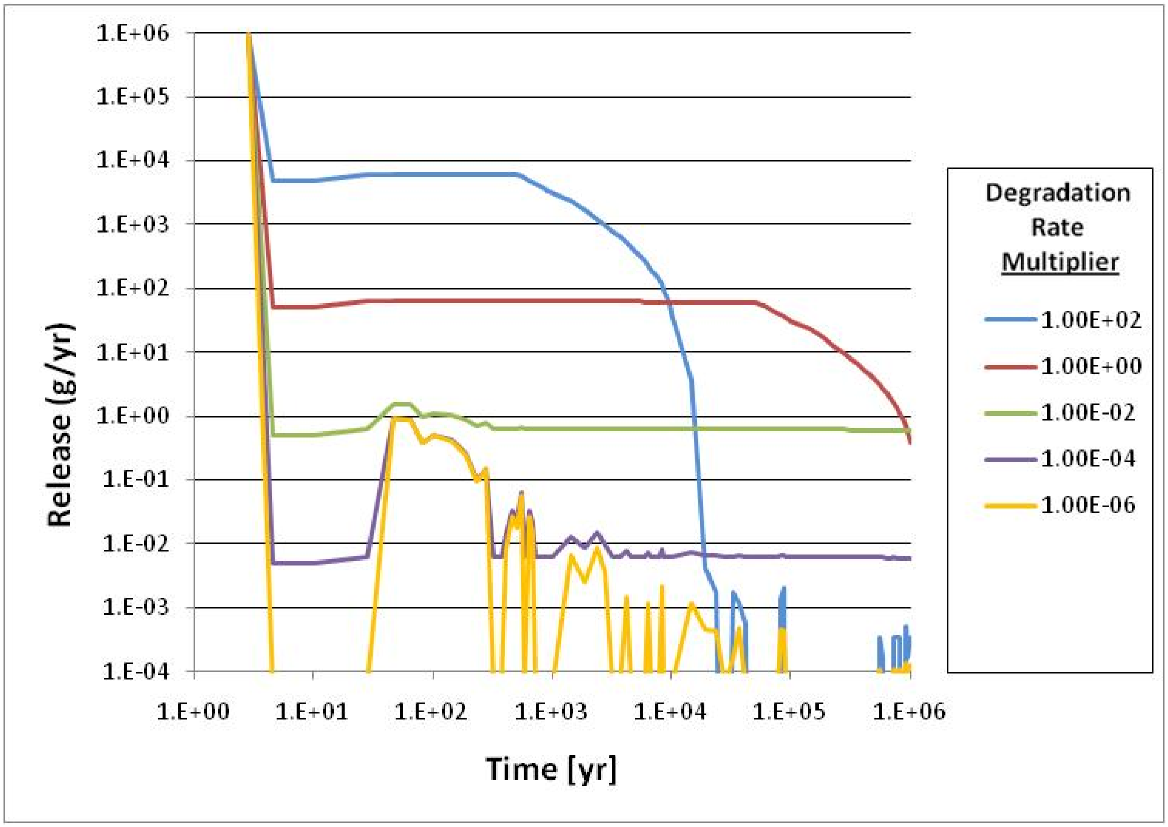


Figure D–1. Waste Form Release Rate for I-129

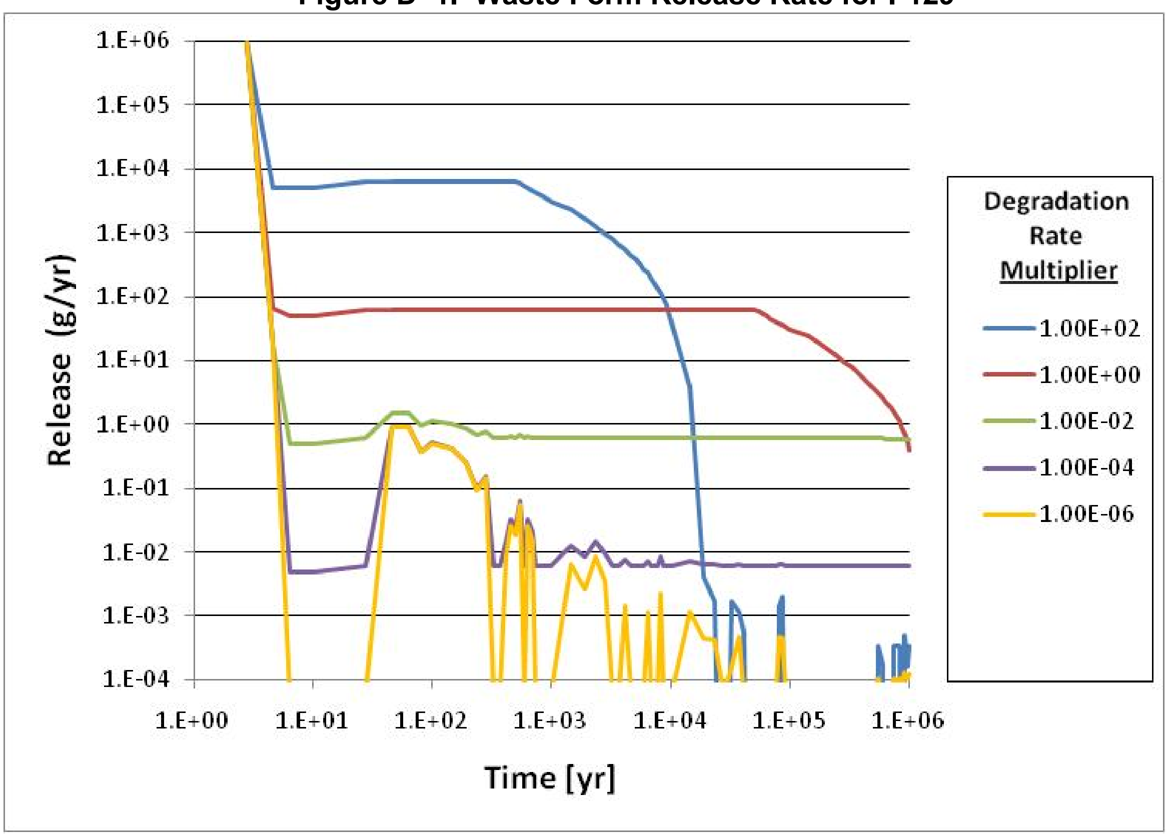


Figure D-2. Release Rate from Backfill (Zone 2) for I-129

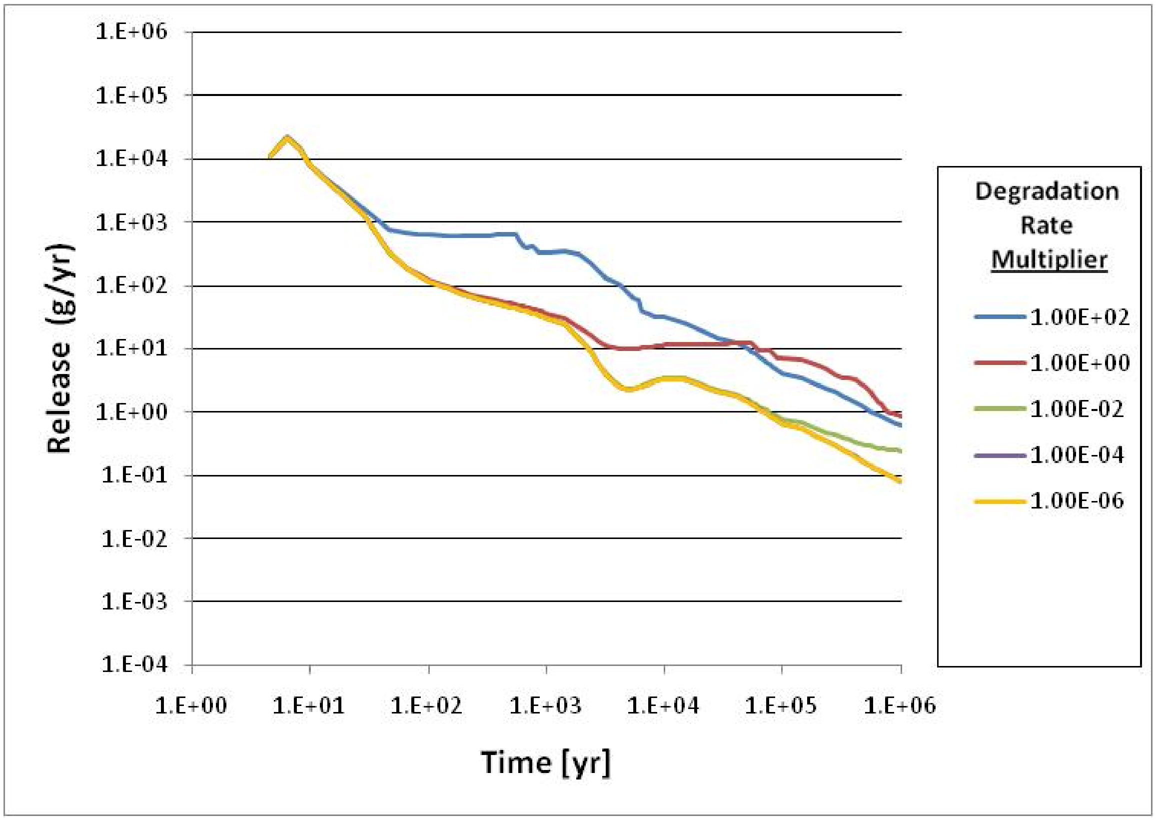


Figure D-3. Release Rate from Far Field Leg 3 for I-129

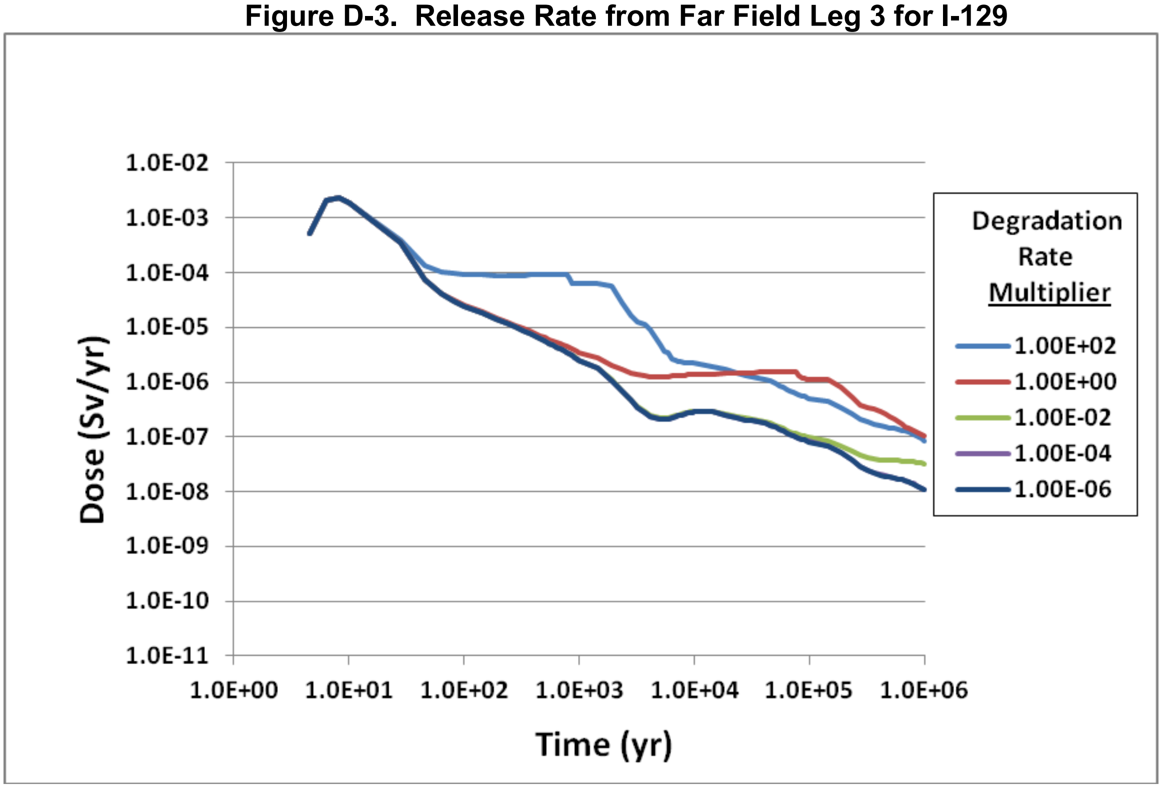


Figure D–4. I-129 Dose

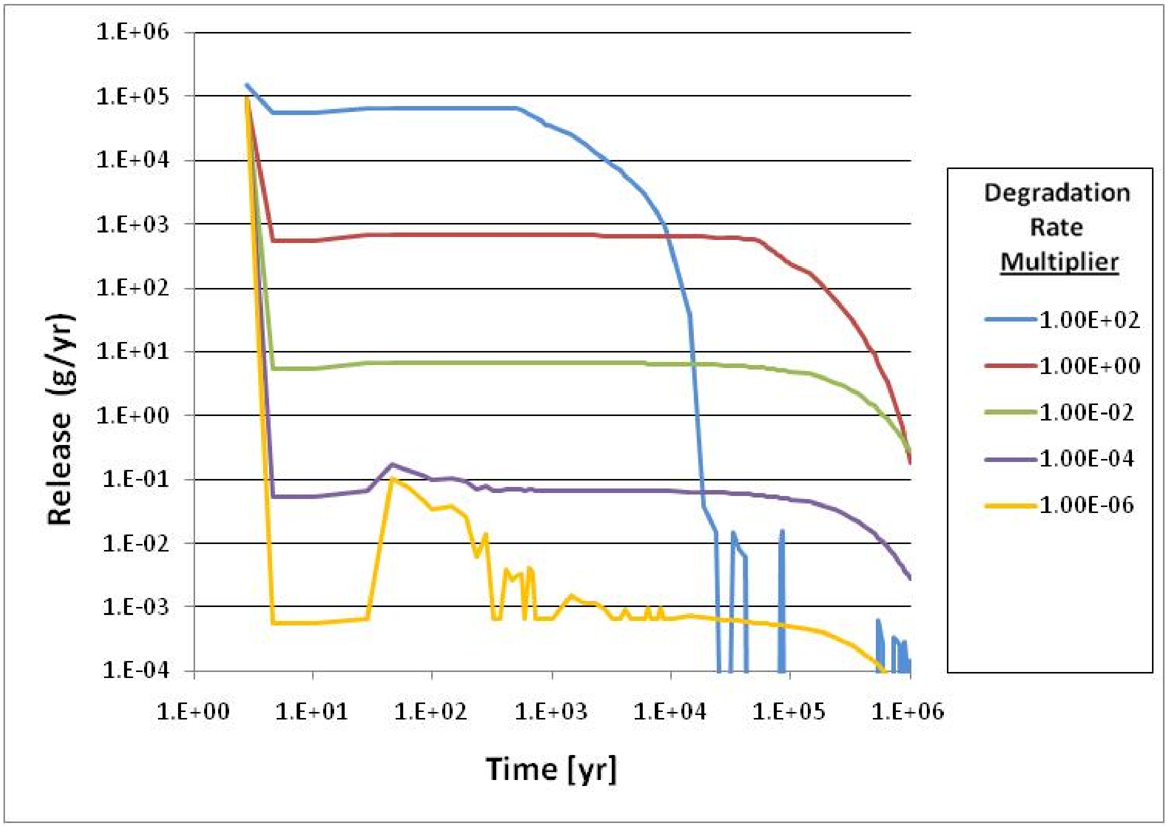


Figure D–5. Waste Form Release Rate for Tc-99

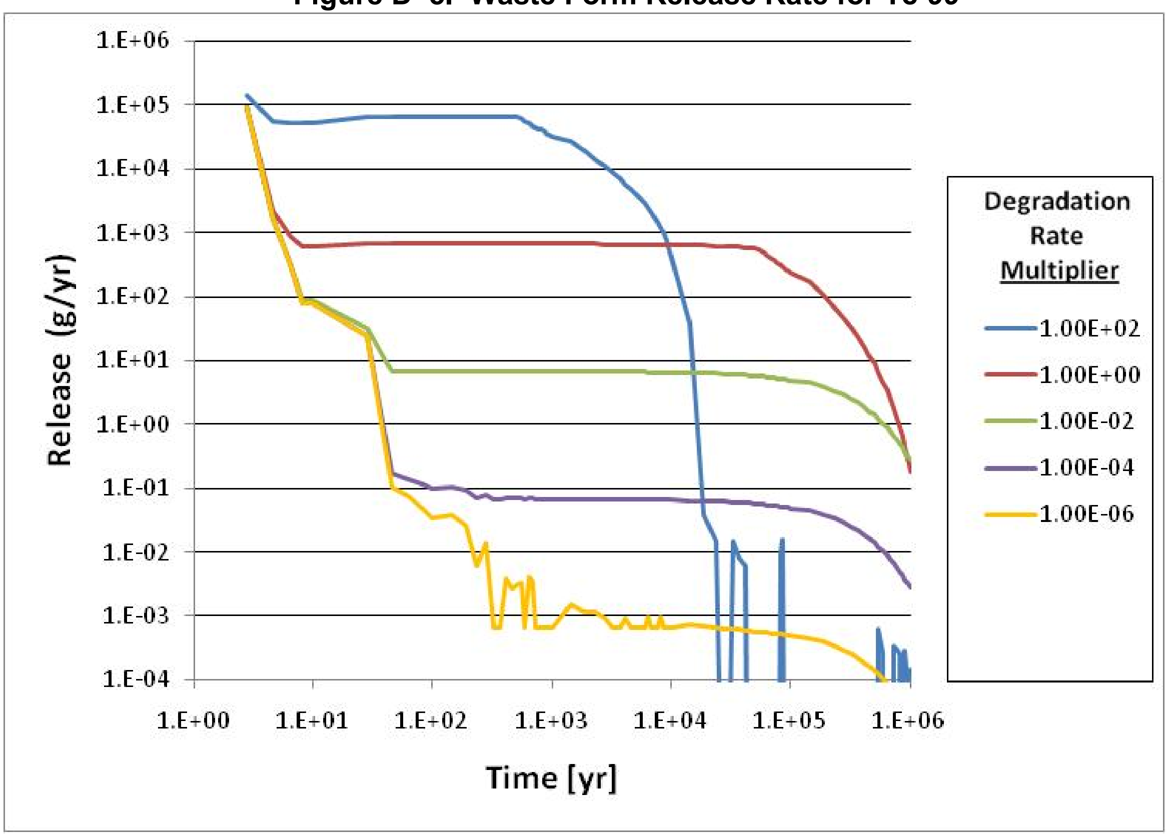


Figure D-6. Release Rate from Backfill (Zone 2) for Tc-99

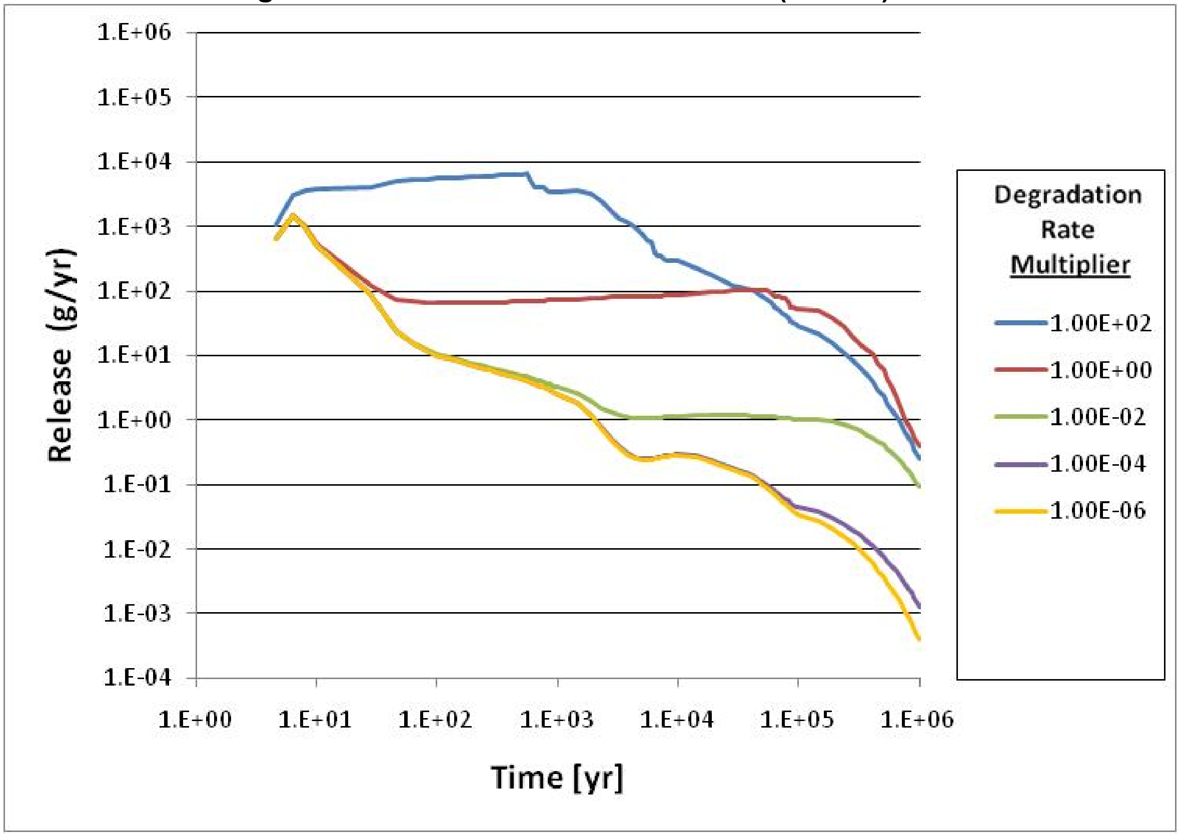


Figure D-7. Release Rate from Far Field Leg 3 for Tc-99

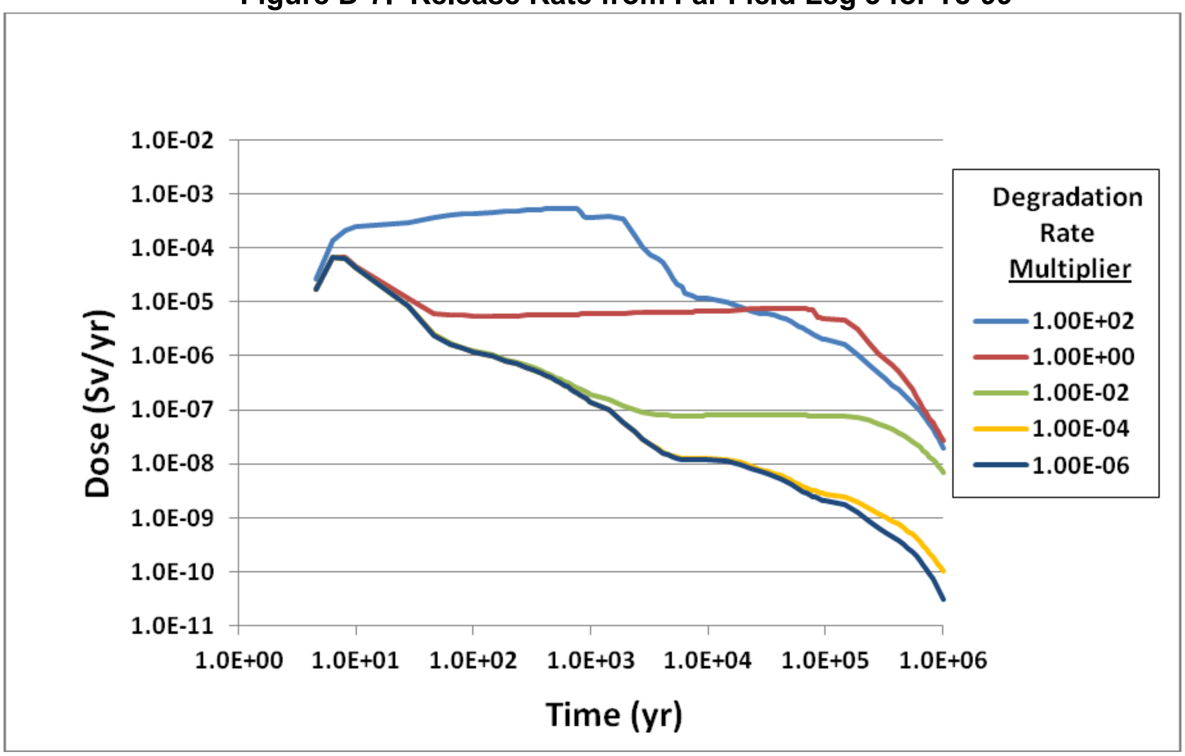


Figure D–8. Tc-99 Dose

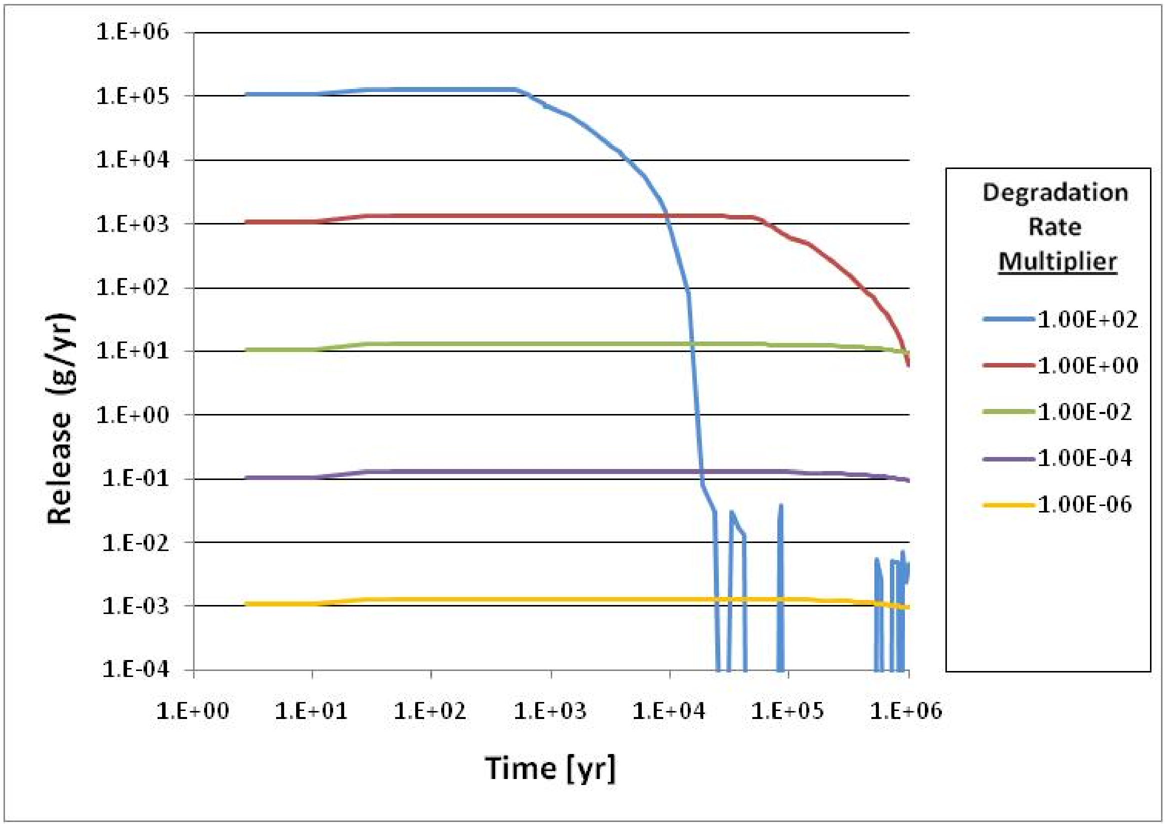


Figure D–9. Waste Form Release Rate for Np-237

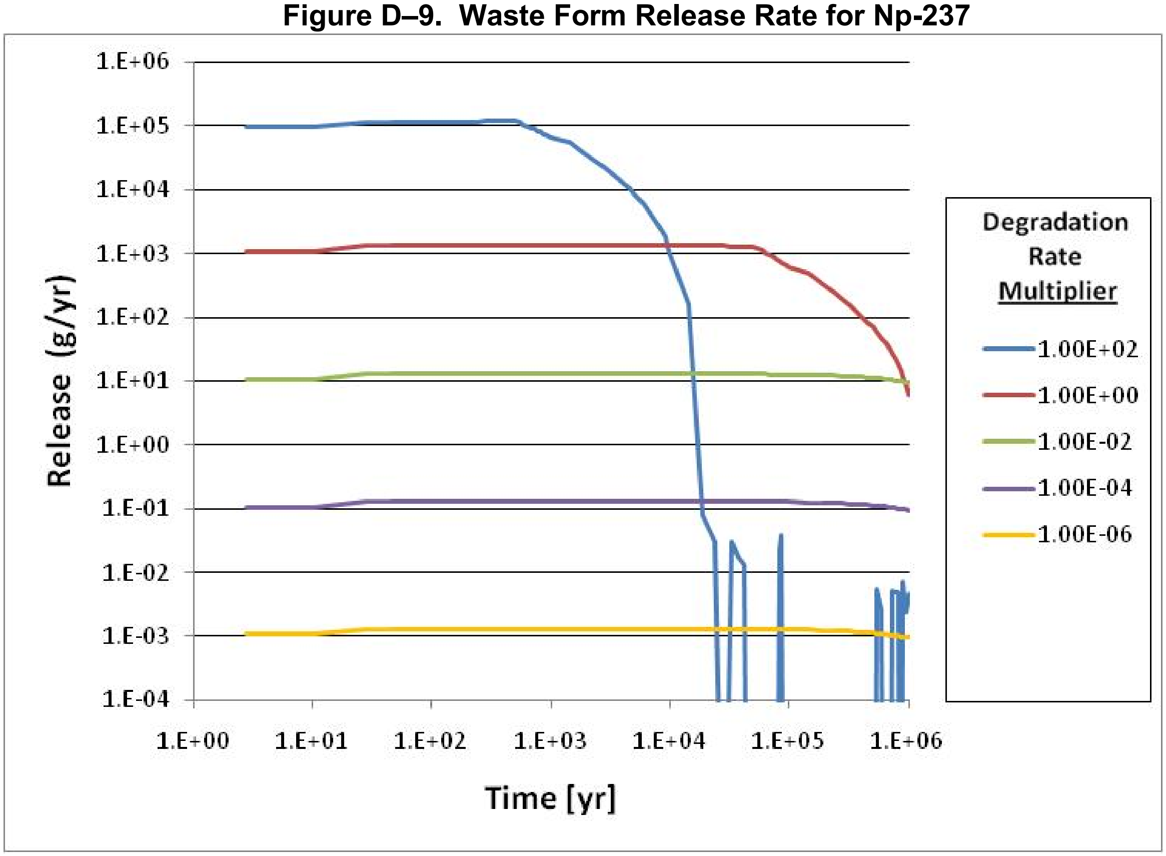


Figure D-10. Release Rate from Backfill (Zone 2) for Np-237

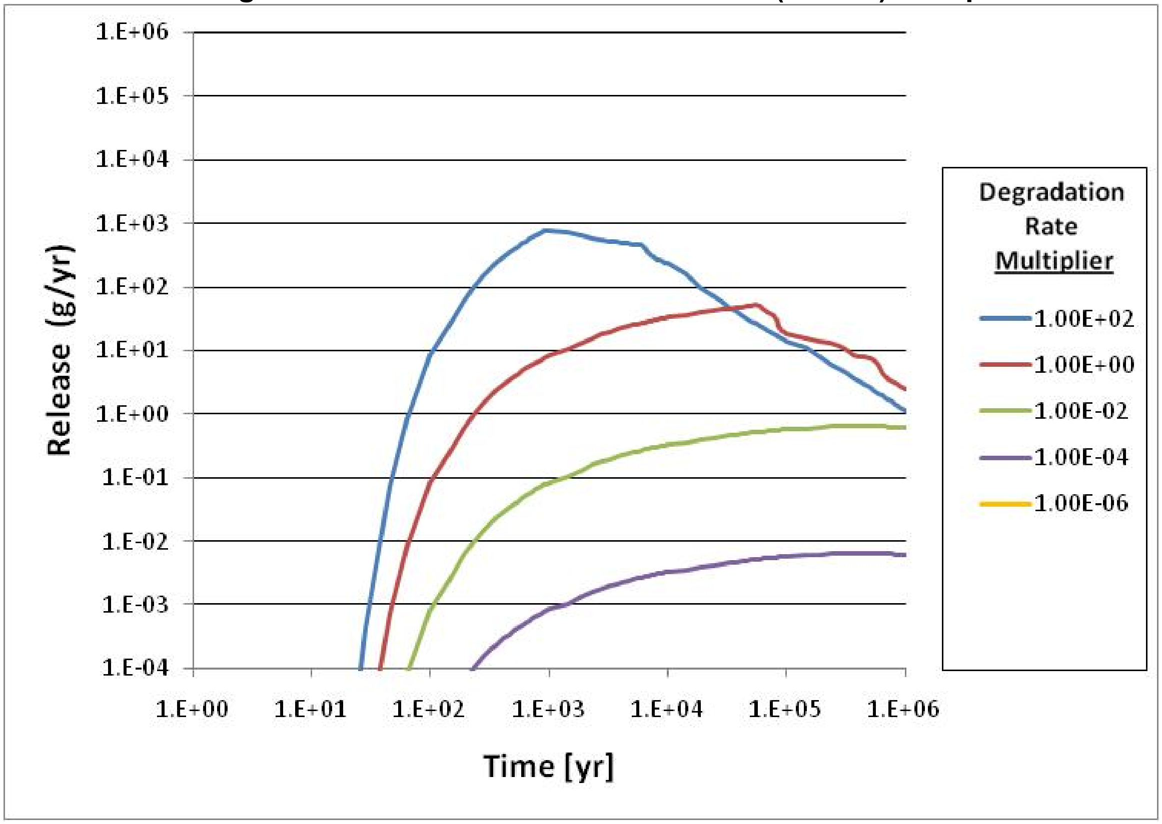


Figure D-11. Release Rate from Far Field Leg 3 for Np-237

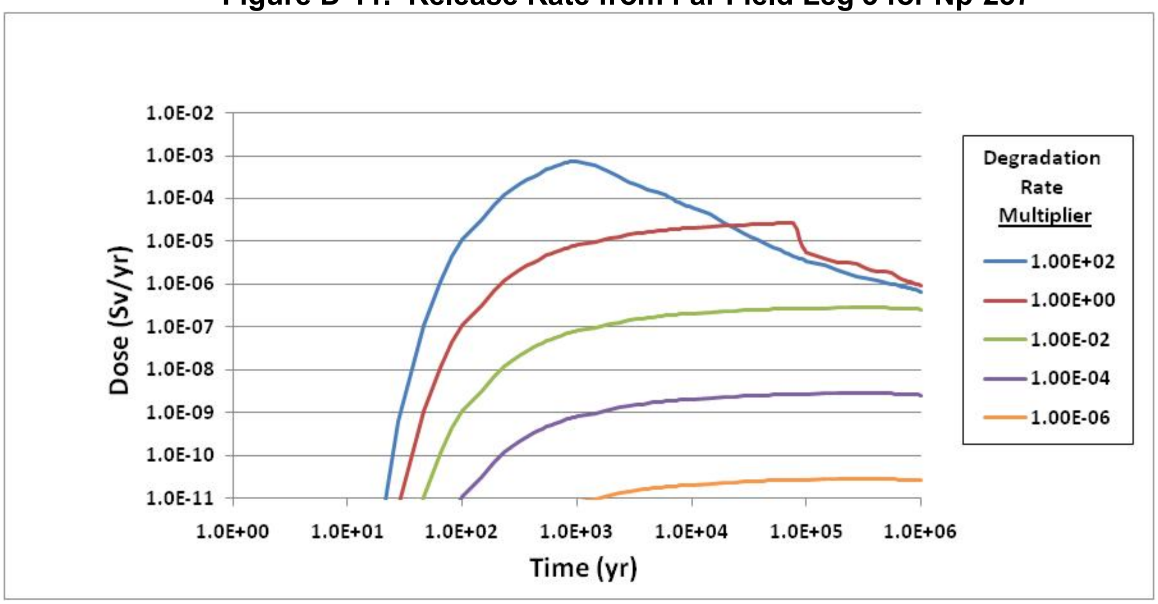


Figure D–12. Np-237 Dose

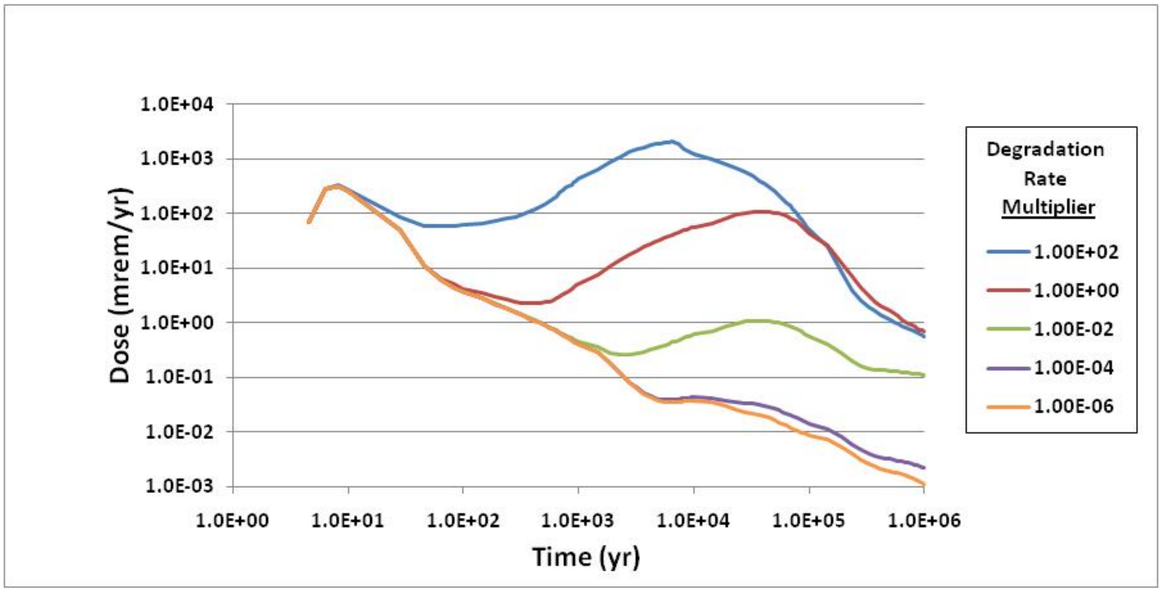


Figure D–13. Total Dose