

# **Performance Assessment: A Model for Scoping of Options and Analyzing Risk, Beta Version (β-SOAR)**

## **User Guide**

*Jointly Prepared By*

**The U.S. Nuclear Regulatory Commission and  
The Center for Nuclear Waste Regulatory Analyses  
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## EXECUTIVE SUMMARY

This user guide describes the operation and capabilities of the *beta-Scoping of Options and Analyzing Risk* (β-SOAR) model. This 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. It was developed over an approximately four-month period by the NRC staff 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 β-SOAR model. The beta (β) designation in the name indicates this initial version of the model and the assigned default input parameters are considered preliminary and have yet to undergo rigorous review and validation. Hence, application and results from the current version of β-SOAR should be used with caution.

Public expectations and acceptance of any HLW disposal site cannot be achieved without technical and ethical trust of 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 β-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 high level waste. 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 waste disposal, (ii) responding to inquiries from Congress, the Commission, the public, and the U.S. Department of Energy's (DOE) Blue Ribbon Commission (BRC.gov), (iii) preliminary identification of potential risk and performance insights for a range of geologic disposal options for high-level nuclear waste (e.g. granite, clay, alluvium), 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. Note that the β-SOAR is not intended to be used as a licensing tool. The β-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: U.S. Nuclear Regulatory Commission. 2010

## 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 their 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 extent, 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 in order 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 three and four. Based on the current uncertainty in the national policy for high-level waste 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 Beta Scoping of Options and Analyzing Risk Model

Under development by the U.S. Nuclear Regulatory Commission (NRC) is a beta (preliminary) version of a performance assessment model named *beta-Scoping of Options and Analyzing Risk* (β-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 high-level waste disposal options. These insights will support development of a regulatory framework in an evolving regulatory environment for licensing and regulating permanent disposal of high-level waste. 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. The beta (β) designation in the model name indicates that this initial version of the model and the assigned default input parameters are considered preliminary and have yet to undergo rigorous review and validation. Hence, application and results from the current version of β-SOAR model is intended to be applied for scoping analyses and should be used with caution. Some specific limitations of the β-SOAR are discussed in Section 2.2.2.

Considering the current uncertainty in the U.S. national policy for high-level waste disposal, the initial version of the β-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 its contractors, 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 described in greater detail 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 β-SOAR model will be used to assist the NRC staff to focus its evolving regulatory program for high-level waste 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 the β-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 require different calculations for risk assessment. Accordingly, the modular structure and analytic approach of the model is

designed to accommodate additional complexity and more detailed process-level models in future revisions.

### **1.3 Objectives**

The objectives of the β-SOAR model are to

- 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 high-level waste disposal options.
- Develop the tool in such a way that provides the technical staff an efficient and effective computational tool for future expansion or implementation of alternative approaches.

As indicated above, the need for 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 β-SOAR User Guide are to

- Provide an overview of the conceptualization of the β-SOAR model (the bases, equations, input, output, assumptions, etc).
- Provide an overview of the modeling environment, key flexibilities of the β-SOAR model, and general guidance for using the model.
- Provide an overview of the key aspects of the β-SOAR components.
- Summarize activities conducted to provide confidence in the β-SOAR results (Fiscal Year 2011 activity).
- Summarize key risk and performance insights derived from model development and execution (Future Activity).
- Identify data and analytic modeling needs to support an independent confirmatory capability for the regulatory program (Future Activity).



## 2 OVERVIEW OF β-SOAR

### 2.1 Contents of β-SOAR

#### 2.1.1 System Overview

The β-SOAR model approximates performance of a generic geologic nuclear waste disposal system. Figure 2-1 illustrates the general conceptual model considered by β-SOAR. The engineered portion of the system comprises waste form, waste package, and engineered backfill material. The waste form may be specified in terms of different combinations of commercial spent nuclear fuel (SNF), high-level waste glass, and spent mixed-oxide (SMOX) fuel, which degrade at different rates. The model considers potential failure of waste packages by two concurrent mechanisms: 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 mechanisms allow for flexibility to represent different waste package materials and failure mechanisms. Radionuclides released from degraded waste forms may migrate out of the waste package, through a backfill region, and into the surrounding natural system. The natural system is represented by three “legs” for which characteristics are specified to represent transport pathways through up to three different geologic media. The length of each transport leg can be defined by the user. Radionuclide transport through each leg can be either through a porous rock or a fractured, low-permeability rock. 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 exposure pathways during the simulation period.

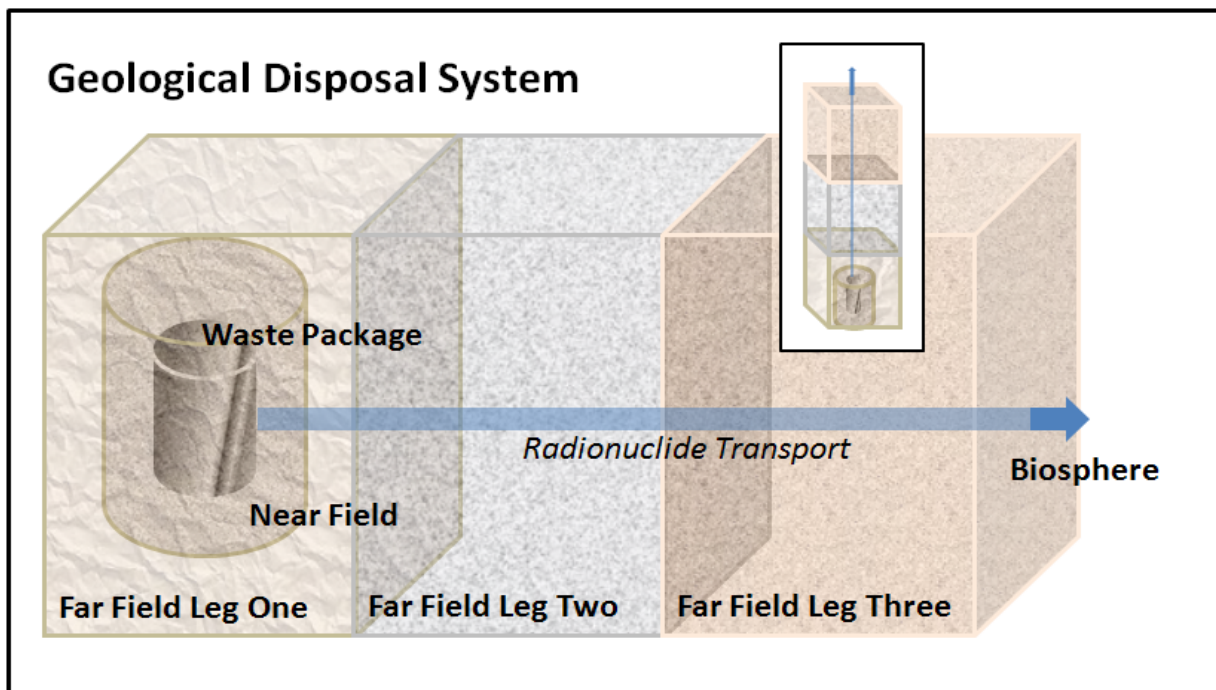


Figure 2-1. Schematic Illustration of Disposal System Modeled in β-SOAR. The Waste Form Is Considered To Be Inside the Waste Package.

### 2.1.2 Component Overviews

The key model components of the β-SOAR model are

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

Brief descriptions of these model components are provided in the following paragraphs. More detailed descriptions of the computational approaches and input parameters for each of the five model components are summarized in Chapter 4.

The β-SOAR Waste Form model component has the capability to estimate of up to three types of waste forms: commercial spent nuclear fuel, high-level waste glass, and spent mixed-oxide fuel. The total inventory and relative amounts of each waste form can be defined by the user. Both bound and unbound radionuclide inventories can be considered, and may be released from a waste package after a waste package breach. Bound radionuclides are those that are trapped inside the waste form matrix (e.g. glass) and are not available for transport until the waste form matrix degrades. Unbound radionuclides are not trapped inside a waste form matrix and are instantly available for transport and may represent gap and grain boundary radionuclides. Waste form degradation is conceptualized to occur at a constant rate, which is calculated based on the type of waste form and chemical environment.

The β-SOAR Waste Package model component has the capability to assess two modes of waste package failure. The first mode considers failure as a distribution over time (e.g., uniform or normal distribution of failures with respect to time). This time-distributed failure mechanism is used to approximate general (uniform) corrosion that progresses slowly over time. The second failure mechanism implements failures as a step function over time (e.g., 10 percent of waste packages fail at a specific time). This failure mechanism is used to approximate the effects of localized corrosion, which affects only certain materials, but may progress rather quickly 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. With appropriately modified inputs, the computation of failure timing and breach area could be modified to approximate additional failure mechanisms, such as stress corrosion cracking and mechanical damage.

The β-SOAR Near Field model component has the capability to assess advective and diffusive radionuclide releases through a breach in the waste package, a surrounding diffusive barrier, and a zone of surrounding host rock that leads to a flow path in the far field. The diffusive barrier is used to represent engineered backfill and its presence or absence can be specified by the user.

The β-SOAR Far Field model component has the capability to represent radionuclide transport through groundwater pathways in the natural system. The term far field refers to the potential for radionuclides to be transported far away from the engineered and disturbed zones represented by the near field. The far field in β-SOAR 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

have either fracture-dominated (e.g., granite) or matrix-dominated (e.g., alluvium) transport pathways. The length of each transport leg can be defined by the user.

The β-SOAR Biosphere model component has the capability to assess dose to a hypothetical person (receptor) who drinks groundwater from a well that captures all or part of the 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**

Initial versions of performance assessments are usually based on a detailed scenario analysis for a specific location. Because the β-SOAR is a scoping tool for developing 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 in different combinations.

### **2.2.2 Model Limitations**

Comparison of the β-SOAR to the Nuclear Energy Agency (2006) features, events, and processes list identified certain features, events, and processes that are not explicitly included in the model. Note that exclusion of certain features, events, and processes from this initial version of the model was not based on any specific knowledge or bias. The model retains flexibility to consider additional features, events, and processes in future versions. The following potentially significant processes are not currently included in this initial version of the β-SOAR:

- The β-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 the nearest groundwater flow path. 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 in a variety of applications.
- The β-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 applications is found to be a dominant pathway.
- The β-SOAR model does not explicitly include the influences of thermal heat on the surrounding environment generated by the decay of radioactive. This includes the mechanical integrity of the host rock.

## β-SOAR USER GUIDE

- The β-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 in backfill and the geologic host media. Consideration of alternative geochemical environments can be estimated by comparing model results for alternative parameter sets developed for specific geochemical environments. The initial model version presented in this report includes alternative parameter sets intended to provide the users a choice of oxidizing or anoxic geochemical environments in fractured granite or porous media.
- The β-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 applications.
- The β-SOAR model does not explicitly represent dynamic disruptive events, such as seismicity or volcanism. It is possible, however, to modify input parameters and functions to implicitly consider how such processes might affect waste disposal. For example, time-dependent functions describing waste package corrosion or waste form degradation can be modified to account for the more pronounced thermal effects early in the disposal period. Using modified inputs to represent thermal effects or disruptive processes requires careful offline analysis by qualified users.
- The β-SOAR model assumes no nuclear criticality event (i.e., nuclear fission reaction) that could occur during the performance period.
- The β-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 are explicitly represented.
- The β-SOAR model does not model complex groundwater flow and transport processes (e.g., splitting of flow paths, time-varying velocity, or geochemical conditions).

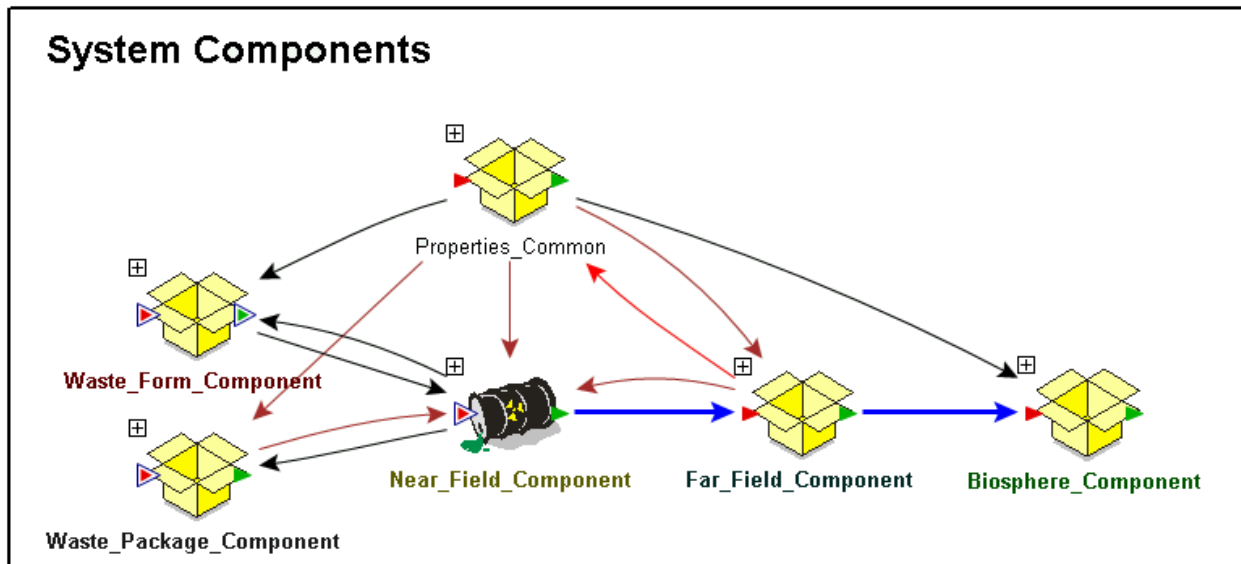
## 3 OVERVIEW OF MODEL ARCHITECTURE

### 3.1 Model Structure

The β-SOAR model is composed of five component models that were developed using GoldSim probabilistic simulation environment software. The GoldSim simulation environment permits modular, object-oriented model architecture with the benefit of being able to visualize connections between model elements. The five main model components (waste form, waste package, near field, far field, and biosphere) are each developed in separate GoldSim “containers” as illustrated in Figure 3-1. These components were developed modularly to facilitate potential future modifications. For example, if a more detailed waste package model is desired, changes can be made to that specific container with minimal impact on the other model components. By clicking on the component containers, the user can view the contents of the container used to develop the model component calculations. Users not familiar with the GoldSim environment should consult the GoldSim user manual (GoldSim Technology Group, LLC, 2010a) for descriptions of the various types of GoldSim elements. Following is a brief introduction to the model components, as packaged in the β-SOAR. See the corresponding section for each model component in Chapter 4 for additional details.

The Waste Form model component includes the radionuclide inventory and the waste form degradation rates. As packaged, the waste forms that can be approximated are spent nuclear fuel, high-level waste glass from reprocessed spent nuclear fuel, and spent mixed-oxide fuel. Both oxidic and anoxic degradation rates are considered.

The Waste Package component includes the type of waste package material, the chemical degradation mechanism, and the potential opening areas when failure occurs. The waste package materials approximated in this initial version of the model are copper, stainless steel, carbon steel, and titanium. The main degradation process implemented is the general corrosion algorithm, which computes corrosion failures for either oxidic or anoxic environments, as selected



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

by the user. Localized corrosion is implemented for certain materials depending on their localized corrosion occurrence tendency.

The Near Field component includes the characteristics of and radionuclide transport through the waste package internals, any surrounding backfill, and the disturbed zone within the geologic host formation. Transport lengths of each of the three zones can be specified by the user. In this initial version of the model, the assigned properties of the backfill zone are for a bentonite backfill, for which diffusion is expected to be the dominant transport mechanism. The user specifies properties of the surrounding disturbed zone to be either fractured granite or a porous medium.

The Far Field component includes the geologic media and the radionuclide transport pathways of the natural system. The geologic media were selected to encompass the range of dominant transport pathways. The pathway end-members are matrix dominated and fracture dominated. 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. For the β-SOAR, the biosphere is limited to a drinking-water ingestion pathway.

### **3.2 Model Flexibility**

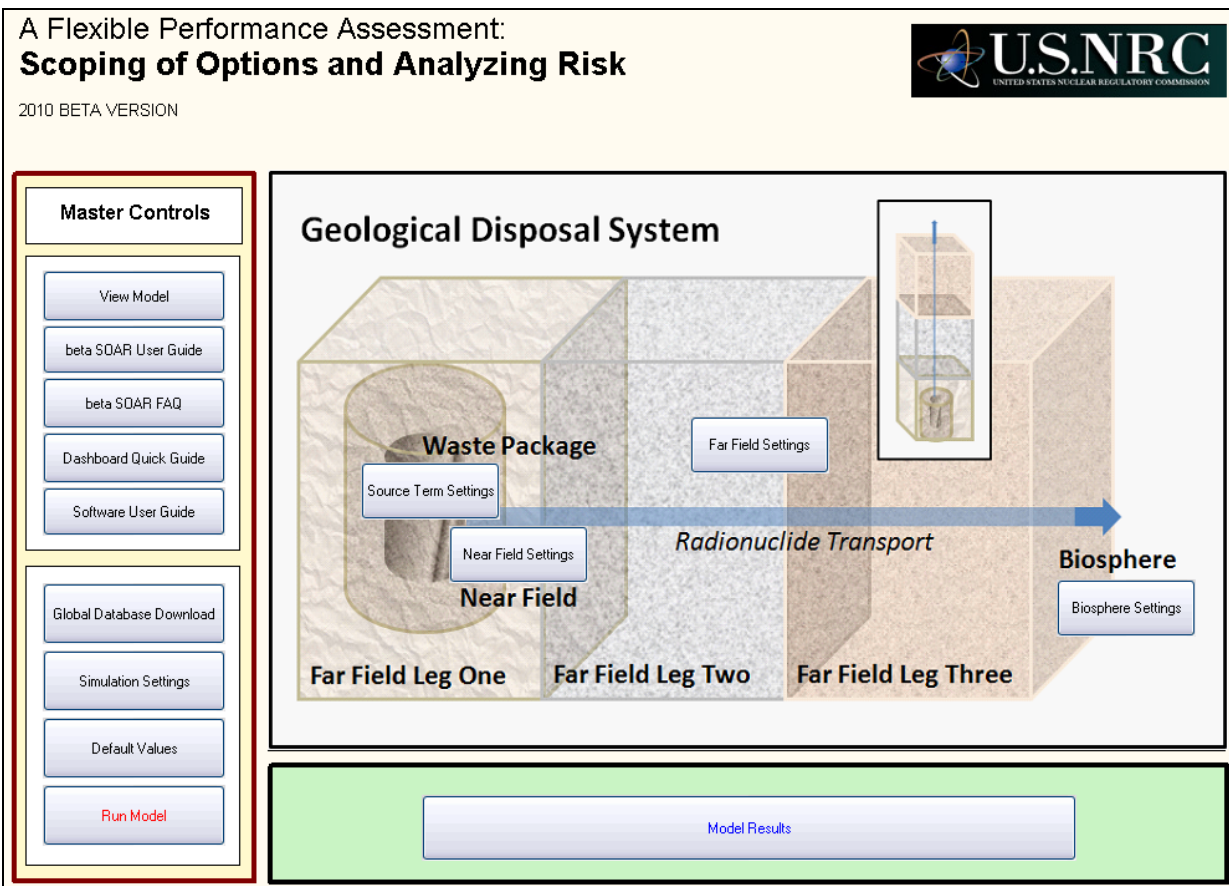
Three levels of model flexibility were incorporated into the β-SOAR and are a function of the level of modifications required to implement the model. Level-one flexibility is represented by the user-selected parameter options on the “dashboard” interface of β-SOAR (see Figure 3-2). Level-two flexibility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

#### **3.2.1 Level-One Flexibility: GoldSim Dashboard Variables**

Level-one flexibility is incorporated into the initially parameterized version of the β-SOAR. To exercise the level-one flexibility, the β-SOAR has a dashboard that allows a limited set of parameter combinations to be considered for simulations. Figure 3-2 shows the overall layout of the β-SOAR main dashboard. As shown in the figure, the dashboard provides access to level-one parameter settings for Source Term (includes both Waste Form and Waste Package parameters), Near Field, Far Field, and Biosphere. Selecting one of these options takes users to a menu of level-one parameters that can be modified using the dashboard. The level-one parameters permit the capability to simulate 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 free GoldSim Player software, which can be obtained from <http://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 β-SOAR are listed and described in Appendix A. Modification of these default values requires use of the GoldSim Probabilistic



**Figure 3-2. The β-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**

Simulation Environment software and cannot be accomplished with the free GoldSim Player software. To change model default parameter values, users need to locate the parameter distribution within the model and revise the parameter 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 β-SOAR: physical and parametric. Physical-based model inputs are based on some scientific basis or measurable quantity, such as metal corrosion rates. Parametric-based model inputs are more flexible, such as generic enhancement factors used to account for conceptual uncertainties that are not easily quantified by data.

For an example of a physical-based model input modification, a user may obtain corrosion rates for a specific titanium alloy. The user could use the GoldSim software to modify the corrosion rates currently in the β-SOAR.

For an example of a parametric-based model input modification, the user may decide to use a scaling fraction to compute the cross section of the transition region from the backfill material to the closest fracture, using the backfill unit cross section as reference. The user could use the GoldSim software to modify a waste form degradation-rate multiplier. The value could be

decreased to account for cladding protection or increased to account for damage to the waste form in transport to the disposal system. Another example is that modification of the waste package failure distribution and breached area could approximate a disruptive event if that capability is desired in future versions of the model. Note that any such parameter modifications should have an appropriately developed technical basis.

### **3.2.3 Level-Three Flexibility: Modification of Model Structure**

Level-three flexibility involves modification of the model structure. This can occur through the addition or subtraction of model inputs. For example, a user may develop a submodel that explicitly tracks radionuclide transport through a large fracture network. The user could create this submodel and incorporate it into the β-SOAR. Modification of model structure requires use of the GoldSim Probabilistic Simulation Environment software, significant experience developing models within the GoldSim framework, and expertise in the process that the model modification is intended to represent.

## **3.3 The GoldSim Modeling Environment**

The β-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 visually see model influences. The simulations use a Monte Carlo approach to explicitly account for uncertainty in model inputs such as waste package corrosion rates or radionuclide sorption coefficients. Additionally, GoldSim calculates radionuclide ingrowth and decay. For system requirements and additional information about GoldSim, please see the GoldSim User Guide (GoldSim Technology Group, LLC, 2010a).

GoldSim allows developers to create a “dashboard” that allows novice users the ability to run simulations of the β-SOAR model. The developer creates a simplified user interface and defines the parameters that a novice user may manipulate. The dashboard can be run on a GoldSim viewer, called the GoldSim Player, Version 10.0 or higher; this software is available as a free download from <http://goldsim.com>. The dashboard, shown in Figure 3-2, allows users to easily access the level-one flexibility in the β-SOAR. Note that β-SOAR includes links on the dashboard to more detailed instructions on use of the dashboard.

The β-SOAR model was generally developed using simplified models and/or abstractions to represent key features, events, and processes associated with geologic disposal. Because of specific modeling needs, however, the implementation of some processes may be slightly more complex. GoldSim has the capability for significant, in-model documentation. Where appropriate in the β-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. The β-SOAR uses this feature by linking to a controlled Microsoft Access database, FPA-SOAR.mdb. Note that in the β-SOAR, only physical-based parameters are controlled via the database.



### 3.4 Quick Start Guide

Perhaps the easiest way to become familiar with and learn to use the β-SOAR model is to open the model and begin exploring from the model 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. Level-one users (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. Level-two and level-three users (Sections 3.2.2 and 3.2.3) must work with a *.gsm* file format, which requires access to GoldSim Probabilistic Simulation Environment software to modify model elements and input parameters not contained on dashboard menus.

Regardless of which model format is used, opening the model will take the user to the 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 Source Term (includes both Waste Form and Waste Package parameters), Near Field, Far Field, and Biosphere. These buttons take the user to the respective input menus illustrated in Figures 3-3 through 3-6. Rolling the mouse cursor over any of the input entries of these dashboard menus will produce a pop-up text box to aid the user with a description of the parameter.

## Source Term

Note that Source Term experiences conditions (redox and rock type) defined in the Far Field Leg One

[Return to Home](#)
[Source Term Settings](#)
[Near Field Settings](#)
[Far Field Settings](#)
[Biosphere Settings](#)

### Waste Form

[View Component](#)

**Waste form proportions tracked in the system:**

Fraction of Waste Inventory that is Spent Nuclear Fuel and Spent Mixed-Oxide Fuel (the remaining fraction is assumed to be High Level Waste): 0.95

Fraction of the Spent Nuclear Fuel that is commercial SNF (the remaining fraction is assumed to be sMOX): 0.5263

	commercial SNF	sMOX	HLW Glass
Inventory Loading Factor	<span style="border: 1px solid black; padding: 2px 10px;">1</span>	<span style="border: 1px solid black; padding: 2px 10px;">1</span>	<span style="border: 1px solid black; padding: 2px 10px;">1</span>
Fraction of WF Initial Inventories Available for Release:	<span style="border: 1px solid black; padding: 2px 10px;">1</span>	<span style="border: 1px solid black; padding: 2px 10px;">1</span>	<span style="border: 1px solid black; padding: 2px 10px;">1</span>
Degradation Rate Multiplier	<span style="border: 1px solid black; padding: 2px 10px;">1</span>	<span style="border: 1px solid black; padding: 2px 10px;">1</span>	<span style="border: 1px solid black; padding: 2px 10px;">1</span>

### Waste Package

[View Component](#)

Waste package material: Copper  
Carbon Steel  
Stainless Steel  
Titanium

Breach area computation method: ? Stepwise (Conservative)  
Weighted Average

Check to define waste package thickness (default values used if unchecked) ☐

Waste package thickness (cm): (only used if above is checked) 1

Number of waste packages: 10000

Distribution of general corrosion rates: ? Normal  
Uniform

Scale of distribution of general corrosion rates: Linear  
Logarithmic

### Initial Radionuclide Mass in Disposal System

C-14	<span style="border: 1px solid black; padding: 2px 10px;">18.5 kg</span>	Tc-99	<span style="border: 1px solid black; padding: 2px 10px;">8.33e4 kg</span>	Pu-239	<span style="border: 1px solid black; padding: 2px 10px;">6.8e5 kg</span>	U-232	<span style="border: 1px solid black; padding: 2px 10px;">0.0563 kg</span>	U-235	<span style="border: 1px solid black; padding: 2px 10px;">3.38e5 kg</span>	All Radionuclides <span style="border: 1px solid black; padding: 2px 10px;">7.83e7 kg</span>
Cs-135	<span style="border: 1px solid black; padding: 2px 10px;">5.45e4 kg</span>	Np-237	<span style="border: 1px solid black; padding: 2px 10px;">2.86e5 kg</span>	Pu-240	<span style="border: 1px solid black; padding: 2px 10px;">4.29e5 kg</span>	U-233	<span style="border: 1px solid black; padding: 2px 10px;">4.99 kg</span>	U-236	<span style="border: 1px solid black; padding: 2px 10px;">2.02e5 kg</span>	
I-129	<span style="border: 1px solid black; padding: 2px 10px;">2.26e4 kg</span>	Pu-238	<span style="border: 1px solid black; padding: 2px 10px;">1.44e4 kg</span>	Pu-242	<span style="border: 1px solid black; padding: 2px 10px;">1.09e5 kg</span>	U-234	<span style="border: 1px solid black; padding: 2px 10px;">9.17e3 kg</span>	U-238	<span style="border: 1px solid black; padding: 2px 10px;">7.6e7 kg</span>	

**Figure 3-3. β-SOAR Dashboard Menu for Source Term Which Includes Configuration Inputs for the Waste Form and Waste Package Model Components**

3-5

# β-SOAR USER GUIDE

Near Field


Return to Home

Source Term Settings

Near Field Settings

Far Field Settings

Biosphere Settings



Note that the Near Field Component experiences conditions (redox and rock type) defined in the Far Field Leg One

View Component

Note that Source Term and Near Field Components experience conditions (redox and rock type) defined for the Far Field Leg One

☐ Bypass the backfill (diffusive barrier)
 ☐ Disable near field advective releases
 ☐ Enable radionuclide sorption in transition region between buffer and far field

Water volume inside the waste package (cubic meters):

Near field flow factor (only used if repository host rock is fractured rock):

Multiplier to define cross section of transition region (region between buffer and far field). The buffer cross section is selected as reference.

Figure 3-4. β-SOAR Dashboard Menu for Near Field Model Component Configuration Inputs

Far Field


Return to Home

Source Term Settings

Near Field Settings

Far Field Settings

Biosphere Settings

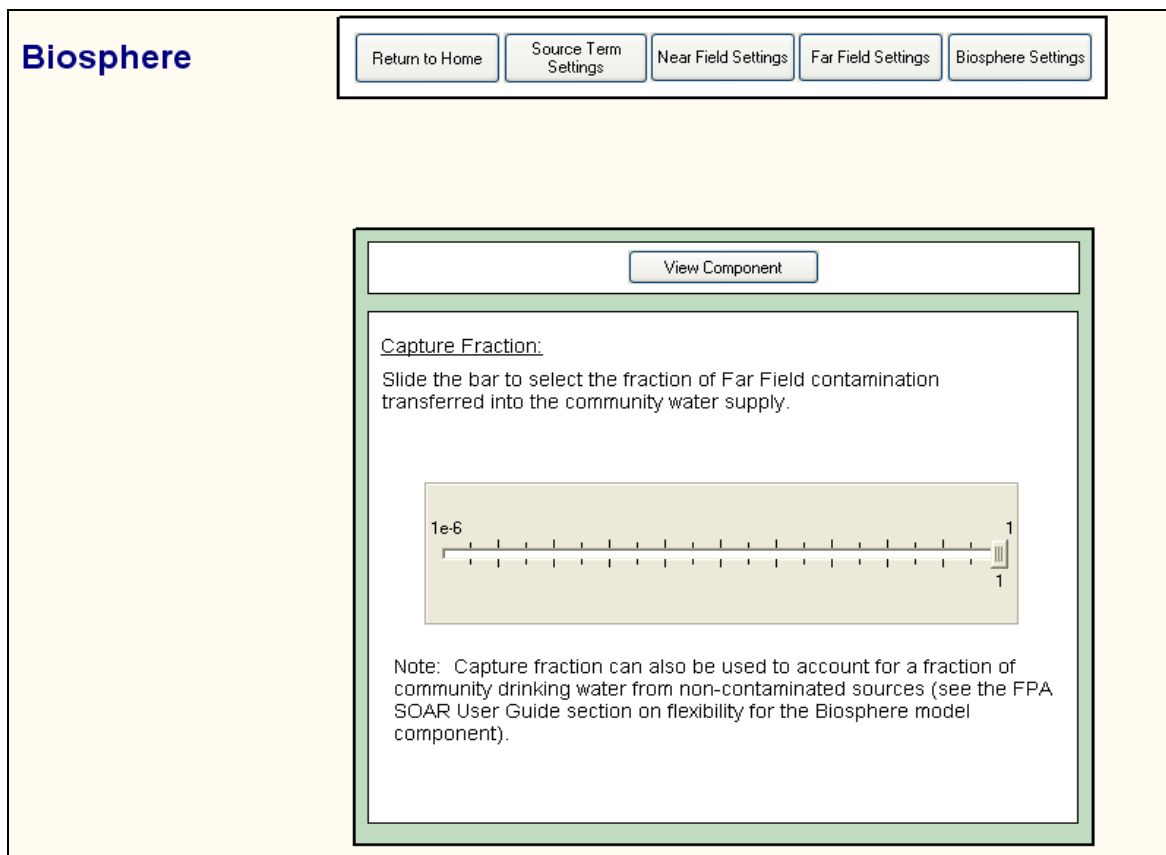


View Component

Note that Source Term and Near Field Components experience conditions (redox and rock type) defined for the Far Field Leg One

Far Field Leg One	Far Field Leg Two	Far Field Leg Three
<div>Flow Result</div> <div>Media: <div>Porous Rock</div><div>Fractured Rock</div></div> <div>Redox: <div>Oxidizing</div><div>Reducing</div></div> <div>Transport length (km): <input type="text" value="1.67"/></div> <div>Effective Porosity Reduction Factor: <input type="text" value="1"/></div>	<div>Flow Result</div> <div>Media: <div>Porous Rock</div><div>Fractured Rock</div></div> <div>Redox: <div>Oxidizing</div><div>Reducing</div></div> <div>Transport length (km): <input type="text" value="1.67"/></div> <div>Effective Porosity Reduction Factor: <input type="text" value="1"/></div>	<div>Flow Result</div> <div>Media: <div>Porous Rock</div><div>Fractured Rock</div></div> <div>Redox: <div>Oxidizing</div><div>Reducing</div></div> <div>Transport length (km): <input type="text" value="1.67"/></div> <div>Effective Porosity Reduction Factor: <input type="text" value="1"/></div>

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



**Figure 3-6. β-SOAR Dashboard Menu for Biosphere Model Component Configuration Inputs**

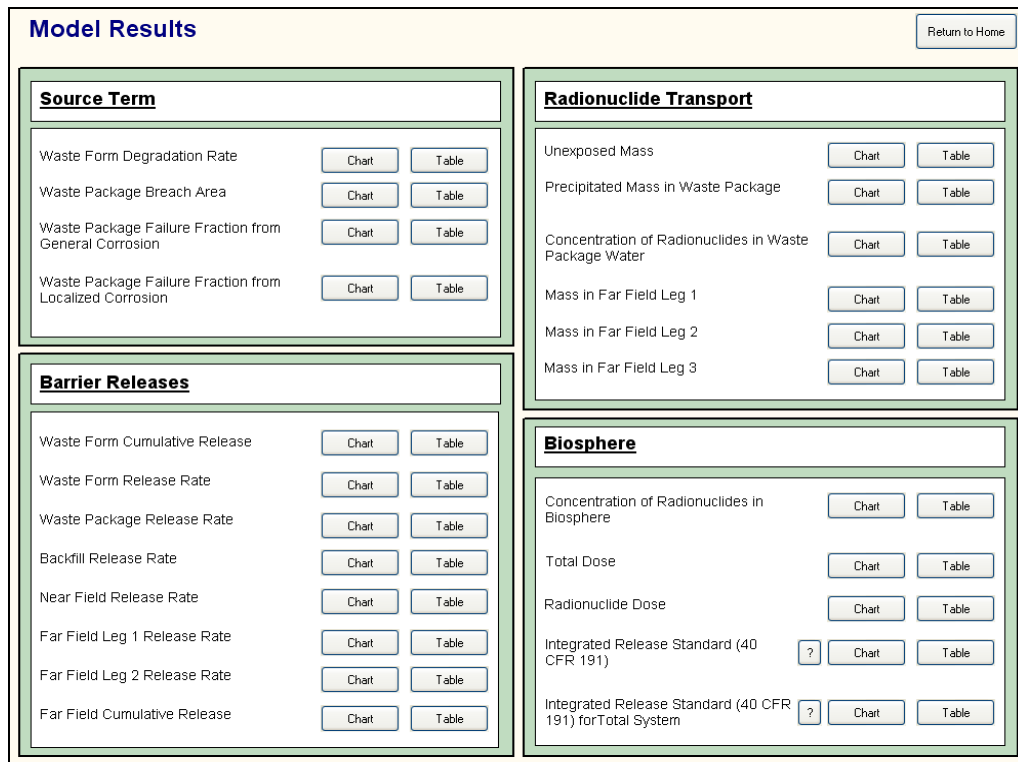
The initial default values for the dashboard parameters can be restored at any time by returning to the main dashboard and clicking the “Default Values” button on the Master Controls panel (see Figure 3-2). If the model has previously been run and has stored results, the model will be in “Results Mode” and the user will not be able to make parameter changes until the model is reset. When working with the GoldSim Player version, resetting the model is easily accomplished 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 3-7). There is no reset option in the full GoldSim Probabilistic Simulation Environment and any changes will result in a new model version. Thus, when working with *.gsm* files users should be experienced with the software and exercise careful version control to avoid making unintended changes to default settings.



**Figure 3-7. GoldSim Player Run Controller Can Be Used to Reset and Run the Model. The “Go” Button Can Be Used To Navigate Into the Individual Model Components.**

After making the desired dashboard 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 the previous model results. If users do not wish to overwrite a previous model, then the model with revised dashboard inputs should 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 3-8. As can be seen in this figure, intermediate and end results for each model component can be viewed in graphical and tabular formats. Tabular results can be saved as separate files for postprocessing or importing to a spreadsheet.



**Figure 3-8. β-SOAR Dashboard Menu for Viewing Model Results**

## 4 MODEL COMPONENTS

### 4.1 Waste Form

#### 4.1.1 Description

The Waste Form model component of the β-SOAR considers the radionuclide mobilization processes from waste form dissolution that affect the source term (i.e., the amount and type of radionuclides released from the waste form for radionuclide transport). The waste forms are emplaced inside the waste package and may be covered by cladding materials (i.e., an outer layer of the nuclear fuel rods to prevent radioactive fission fragments from escaping the fuel 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 the aqueous environment after waste package breaches. The Waste Form model component is integrated 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 time step 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. Fifteen radionuclide species are considered (Pu-238, 239, 240, U-232, 233, 234, 235, 236, 238, Np-237, C-14, Cs-135, I-129, Tc-99). 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, high-level waste glass, and spent mixed-oxide fuel waste forms based on the performance assessment results of various waste forms in both oxidizing and reducing environments (Bechtel SAIC Company, LLC, 2004; Leslie, et al., 2007; Marivoet, et al., 2001). Seven different radionuclide inventories are available, which represent these three distinct waste forms and an additional User-Defined waste form. In the Waste Form model component, all four of these waste forms are proportioned into a single, representative waste form. This representative waste form can then be scaled to represent the total mass of waste forms in the disposal system. Each of the available waste forms has a bound inventory, which requires the specific waste form to degrade before the radionuclides can be dissolved and then released. Each bound radionuclide inventory has a characteristic dissolution rate. In addition to the bound radionuclide inventories, three waste forms (i.e., commercial spent nuclear fuel, spent mixed-oxide, and User-Defined) also include unbound inventories of C-14, Cs-135, I-129, and Tc-99. These unbound inventories are instantly available for transport when the waste package breaches, and are used to model release of these radionuclides more realistically as gap and grain boundary inventories. The β-SOAR has the flexibility to add radionuclides to the inventory if warranted by specific applications.

For the bound radionuclide inventories, the total amount of mobilized radionuclides,  $M$  [g], is calculated as

$$M = m \times I \times t \quad 4-1$$

where  $m$  is the fractional rate of degradation [1/yr],  $I$  is the total inventory of radionuclide [g], and  $t$  is the duration of waste form contacting an aqueous environment [yr]. The fractional degradation rate,  $m$ , is calculated from

$$m = R \times A \quad 4-2$$

where  $R$  is the dissolution rate [g/cm<sup>2</sup>/yr], and  $A$  is specific surface area [cm<sup>2</sup>/g]. The input values of dissolution rate and specific surface area used in the Waste Form model are based on experimentally measured values.

The three distinct waste forms selected are considered to be representative of future waste forms like ceramic and metallic waste forms. These typically have lower degradation rates than high-level waste glass (Wang, 2009; Ebert, et al., 2002). Experimental data on the performance of these future waste forms is limited, however, and has not been 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 three distinct default waste forms, the Waste Form model component assigns default values to the radionuclide inventory, reprocessing effect on inventory, instant release fraction of unbound inventory (i.e., fission and activation products), and fractional rate of waste form degradation. For the User-Defined waste form, the user must assign these values.

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 instant release fraction of unbound inventory and specific surface area of the waste form (Leslie, et al., 2007; Jain, et al., 2004; NRC, 2008).

Radionuclide Inventory: For each of the three distinct waste forms, radionuclide inventories are assigned based on representative values for commercial spent nuclear fuel, spent mixed-oxide fuel, and high-level waste glass in the domestic high-level nuclear waste disposal program. Based on the proportions assigned by the user, the Waste Form model calculates a composite waste form using these representative radionuclide abundances. The literature source of the initial inventory parameter values used in the  $\beta$ -SOAR, which are different for each waste form, assumes 50–100 years of waste form aging occurs before disposal system closure.

Reprocessing Effect on Inventory: To determine the waste form inventory, the user must select the proportions of commercial spent nuclear fuel, spent mixed-oxide fuel, and high-level waste glass. This proportionality is determined in the Waste Form model by first specifying the fraction of total spent nuclear fuel (i.e., both commercial spent nuclear fuel and spent mixed-oxide fuel); the remaining fraction is high-level waste glass. The user then specifies the fraction of spent nuclear fuel that is commercial spent nuclear fuel; the remaining fraction will be spent mixed-oxide fuel. For example, a total inventory of 50 percent high-level waste glass, 10 percent spent mixed-oxide fuel, and 40 percent commercial spent nuclear fuel would use an spent nuclear fuel fraction of 0.5, and then set the fraction of commercial spent nuclear fuel to 0.8. Values of 0 or 1 can be used to create total inventories of only a single waste form.

Instant Release Fraction of Unbound Inventory: For the unbound inventory (i.e., fission and activation products), instant release fractions for commercial spent nuclear fuel and spent mixed-oxide 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 flowing water. For higher burnup (e.g., >60 GWd/MTU) commercial spent nuclear fuel or spent mixed-oxide fuel, the instant release fractions may increase. This approach may lead to higher estimated dose rates at earlier times. Data of unbound radionuclides for these higher burnup waste forms, however, are very limited.

Degradation of Waste Form: The Waste Form model component assumes the bound radionuclides are available for transport at the same rate as the waste form degrades. For commercial spent nuclear fuel, the model considers radionuclides from the bound inventory will be available for transport at the same rate as  $\text{UO}_2$  matrix dissolution (Wilson and Gray, 1990). In an oxidizing environment, the waste form dissolution rate assumes the  $\text{UO}_2$  matrix dissolves electrochemically as soluble species with an aid of oxidants such as dissolved oxygen and hydrogen peroxide (Shoesmith, 2000). In a reducing environment, the waste form dissolution rate assumes the  $\text{UO}_2$  matrix will dissolve chemically as soluble species (Sunder and Shoesmith, 1991). The Waste Form model assumes the degradation rate of spent mixed-oxide fuel can be represented acceptably by commercial spent nuclear fuel degradation rates due to limited data on spent mixed-oxide fuel degradation. This assumption is used to account for uncertainties in available data on spent mixed-oxide fuel degradation and similarities in spent mixed-oxide fuel material properties to those of  $\text{UO}_2$  matrix in commercial spent nuclear fuel. For high-level waste glass, it is assumed that the radionuclides will be available for transport at the degradation rate of high-level waste glass matrix. This rate assumes the high-level waste glass matrix will dissolve chemically, where the process is controlled by concentration of dissolved silica compound in both oxidizing and reducing environments (Bechtel SAIC Company, LLC, 2004).

To determine the fractional degradation rate for each specific waste form, an upper and lower bound for waste form dissolution rate is defined for both oxic and anoxic conditions or 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 are then multiplied by the specific surface area of the waste form, which also accounts for the waste density and surface roughness factors (NRC, 2008). The Waste Form model uses a specific surface area of 0.1 cm<sup>2</sup> [0.04 in<sup>2</sup>] for commercial spent nuclear fuel and spent mixed-oxide fuel (NRC, 2008) and 10 cm<sup>2</sup> [4 in<sup>2</sup>] for high-level waste glass (Bechtel SAIC Company, LLC, 2004). The resulting fractional degradation rates are used to define the upper and lower limits for log-uniform distributions, which are sampled in each realization to represent the fractional degradation rate for each waste form.

In the Waste Form model, the fractional degradation rate of waste form assumes a constant dissolution rate and constant specific surface area over time. This 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 and environmental conditions. 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 reduce uncertainties. In connection to the waste package failure over time, the use of one representative waste package material in the present Waste Package model component assumes that when the waste packages breach, they simultaneously expose all the waste forms present 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. This could lead to different failure times of the waste packages over time, resulting in different 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 spent nuclear fuel, spent mixed-oxide fuel, high-level waste glass, and add a User-Defined waste form. The User-Defined waste form could, for example, consider ceramic or metallic waste forms. To represent the case of potentially higher radionuclide abundances in higher burnup spent nuclear fuel or higher loading high-level waste glass, the user can modify the amount of radionuclides (mass) for each of the defined 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 set aside and 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 by means of 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 fraction of the waste form inventory that is spent nuclear fuel (the fraction of the blended waste form that will be composed of commercial spent nuclear fuel and/or spent mixed-oxide fuel).
- Specify the fraction of spent nuclear fuel that is commercial spent nuclear fuel.
- Specify the values of degradation-rate multipliers for commercial spent nuclear fuel, high-level waste glass, and spent mixed-oxide fuel.
- Specify the releasable fractions of commercial spent nuclear fuel, high-level waste glass, and spent mixed-oxide fuel.
- Specify the inventory loading factors of commercial spent nuclear fuel, high-level waste glass, and spent mixed-oxide fuel.

## **4.2 Waste Package**

### **4.2.1 Description**

The Waste Package model component of the β-SOAR considers the processes that affect the integrity of the waste package. The Waste Package model component specifically



models waste package chemical degradation (i.e., corrosion) processes for some materials in limited environmental conditions. The Waste Package model component is integrated with the Waste Form and Near Field model components. The Waste Package model component calculates waste package failure times and extent of damage to the waste package surface for geologic disposal systems located in either oxidizing or reducing (i.e., redox) host rock, where the host rock type is selected in the Far Field component. Computations in the Near Field model component are also consistent with the redox of the host rock. 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 breached area per failed waste package 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 fractions 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.

Waste Package Specifications: It is assumed the disposal system will consist of a single waste package 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 different corrosion behavior. 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 failures and breach areas.

Failure Mechanisms (General Corrosion and Localized Corrosion): 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 cause failure of a fraction 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

$$t_{gc} = \frac{L}{R_{gc}} \quad 4-3$$

where  $t_{gc}$  is the waste package failure time (yr) by general corrosion,  $L$  is the thickness of waste package material (cm), and  $R_{gc}$  is the general corrosion rate ( $\mu\text{m}/\text{yr}$ ).

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

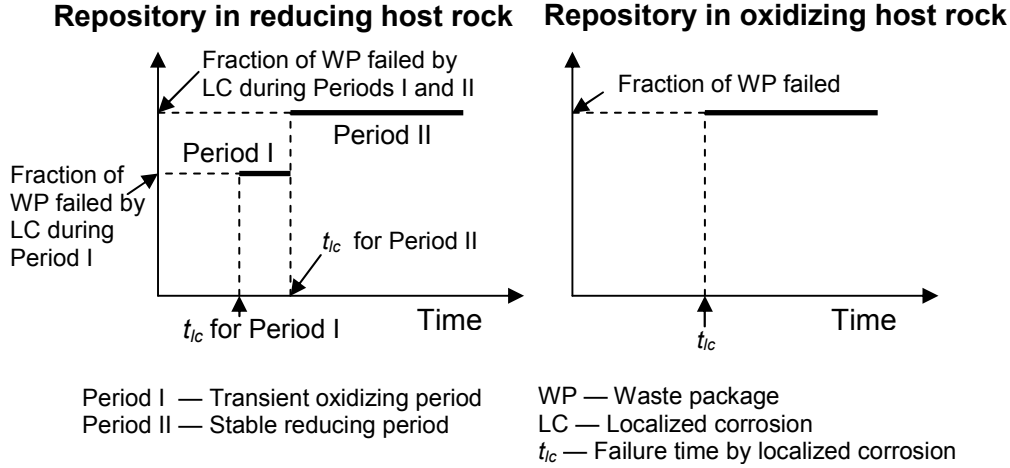
waste package is considered to exhibit a single corrosion rate. The complete distribution of corrosion rates is covered by the multiple waste packages. Thus, waste packages are computed to fail at different times within a realization, depending on their corrosion rate. In the model, general corrosion rates are limited to follow either normal or uniform distributions, or their logarithmic variants, with user-defined low and high bounds. In the case of normal or log-normal distributions, the low and high bounds correspond to the 0.1 and 99.9 percentiles of the failure 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 rates.

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 rock.

For a disposal system located in a reducing host rock, an initial transient oxidizing period (referred to as Period I) is considered prior to the establishment of a stable reducing condition (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 rock is reported to be consumed primarily by 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 the waste packages that did not fail in Period I could exhibit localized corrosion during this period. 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 simulate 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 rock, 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 total waste package breached area 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). The model considers

two distinct breached area fractions: one for localized corrosion and one for general corrosion. For waste package radionuclide release computations, however, a combined breached area per failed waste package is computed at each time step as function of the general and localized corrosion breached area and the number of waste packages failed. Two different approaches in β-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 which the breached area is a constant after failure by localized corrosion. After the waste package with the highest general corrosion rate (or the 99.9 percentile corrosion rate if corrosion rates follow a normal distribution) fails, then the breached area per waste package steps to the larger of the breached area due to localized or general corrosion. In this approach, for systems where both localized and general corrosion occur in the simulation period, the breached area per waste package is overestimated, because waste package failure due to general corrosion is gradual.

In the second approach, the breached area per failed waste package [ $\text{m}^2$ ],  $WP_{\text{breached area}}$ , is computed as a weighted average

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

where  $f_{gc}$  is the fraction of waste packages failed by general corrosion,  $f_{\text{failed WP}}$  is the fraction of waste packages failed,  $f_{gc \text{ breached area}}$  is the general corrosion breached area fraction,  $f_{lc \text{ breached area}}$  is the localized corrosion breached area fraction, and  $A$  is the total area of a waste package [ $\text{m}^2$ ]. 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 are failed by 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, but localized corrosion only affects certain applicable materials.

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 possible 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)].

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  $\beta$ -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, as 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 general corrosion breached area fraction is assumed to be one because general corrosion proceeds uniformly across the entire material surface. On the other hand, localized corrosion is assumed to affect a smaller fraction of the waste package surface area. Other inputs to the Waste Package model component include the waste package surface area [ $A$  in Eq. (4-4)],

which is used to compute radionuclide releases away from the waste package, and the total number of waste packages, which is used to define the total initial inventory.

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 the  $\beta$ -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 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 number of waste packages and 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).
- Specify general corrosion rates, distribution type (normal or uniform), and scale (linear or logarithmic).
- 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 the β-SOAR considers transport of radionuclides from within the waste container, through the disturbed zone outside the waste container, and into the undisturbed natural system. The Near Field component of the β-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, and 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. Each of these zones is discussed next.

In zone 1, two processes are considered. First, dissolved concentrations of radionuclides released from the waste form are computed. For radionuclides with relatively low solubility (e.g., uranium and plutonium) solid phases may precipitate from solution and reduce the dissolved concentration to the solubility limit. Concentrations of highly soluble radionuclides (e.g., cesium and iodine) are not solubility limited and concentrations are limited only by the waste form degradation rate relative to release rate from the waste package. The second process considered in zone 1 is the rate of 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) and concentration difference (diffusive transport), and the cross-sectional area of breaches in the degraded waste package, using the GoldSim cell network representation of the following equation

$$f_{bs} = c_s v + D_s (c_s - c_b) \quad 4-5$$

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

$$D_s = \frac{WP_{breachedarea}}{\frac{L_i}{n_i D_{is} \tau_i} + \frac{L_b}{n_b D_{bs} \tau_b}} \quad 4-6$$

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  $\tau_i$  and  $\tau_b$  are tortuosity of porous medium within mixing  $i$  and  $b$ , respectively. In the β-SOAR it is assumed that  $WP_{breached area}$  includes only general and localized corrosion breach areas. Breach area resulted from stress corrosion cracking is not considered explicitly. Dissolved radionuclide concentrations are limited by solubility; thus, solubility limits impose a constraint on the potential release rates. The solubility constraints on concentration are enforced within the GoldSim mixing cell, which can account for the mass of radionuclides that may have been released from a degraded waste form, but not yet dissolved. 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, the advective release rate will be zero in zone 1 as long as zone 2 is intact (see zone 2 discussion in next paragraph). Diffusive release will occur regardless of the state of zone 2. Therefore, in simulations where backfill degradation is not enabled, diffusive release will be the only mechanism for release from the waste package.

In zone 2, dissolved radionuclides are transported through the engineered buffer or backfill material. The diffusive barrier capability of the backfill may be treated as always intact, degraded over time, or always absent. For an intact zone, radionuclide transport occurs only by diffusion in the direction of the concentration gradient. If degradation over time is enabled, 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 advective radionuclide transport. Advective releases are, therefore, proportional to the fraction of degraded diffusive barriers. For sorbing radionuclides, transport will be delayed by sorption to the buffer material. Solubility constraints are also applied to the radionuclide concentrations in zone 2.

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 if 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 base case) and releases from zone 2 effectively go directly to the far field from zone 2. For fractured host rock, the effective transport distance to the far field flow pathway is computed 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 computed consistently with flow velocities in 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. 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.

Other notable assumptions include

- All sorption of dissolved radionuclides onto solid material occurs instantaneously and is described by an equilibrium partition coefficient ( $k_d$ ) for a specified environment.
- All precipitation/dissolution reactions occur instantaneously and are reversible. A single mineral phase controls the solubility for each element for a specified set of geochemical conditions. All 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 the time of release. If the total concentration exceeds the solubility limit, then uranium minerals from that include proportional amounts of the uranium isotopes.
- The pH, ionic strength,  $p\text{CO}_2$ , and oxidation state do not vary spatially or temporally. 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 system 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 oxic or anoxic conditions. Diffusion coefficients are also radionuclide specific, but are assumed to not be affected by redox conditions.

The base case 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 selecting 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. 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 can be specified through the model dashboard to adjust the near field flow velocity in proportion to the far field flow velocity. 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 β-SOAR 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  $p\text{CO}_2$  by selecting input data sets for either reducing or oxidizing environments. The model also is capable of evaluating degradation of the buffer (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 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 exercise care to 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 β-SOAR considers transport of released radionuclides within the natural-system barrier 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, 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

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

where  $n$  is effective flow porosity [unitless],  $R$  is the retardation factor [unitless],  $c$  is concentration [kg/m<sup>3</sup>],  $Q$  is volumetric flow rate of water [m<sup>3</sup>/yr],  $A_{cs}$  is cross-sectional area [m<sup>2</sup>],  $\alpha$  is dispersivity [km],  $D$  is effective diffusivity [m<sup>2</sup>/yr],  $\lambda$  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

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

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<sup>2</sup>/yr], and  $z$  is distance into the matrix diffusion zone [m].

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

$$R = 1 + \frac{\rho_b K_d}{\theta} \quad 4-9$$

where  $\rho_b$  is the dry bulk density of the porous medium or rock matrix [kg/m<sup>3</sup>],  $K_d$  is the radionuclide-specific equilibrium partition coefficient [m<sup>3</sup>/kg], and  $\theta$  is the saturated porosity of the porous medium or rock matrix [unitless].

The Far Field component provides the capability to treat flow in each transport leg as either a porous medium or a fractured medium. Model parameters used in the transport calculations depend on the medium selected. For calculating water flow rates in a porous 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 the 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 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 above computational approach include

- 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 ( $\alpha$ ) is assumed to be scale dependent and is calculated as a fraction of the transport path length (e.g., 10 percent in the base case 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 non-flowing 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 calculated matrix diffusion flux using the slab geometry with no skin zone is enabled.
- Some radionuclides can be sequestered onto the surface of solid particles for long periods of time, in a process called 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 kinetics). This fixed ratio is described by the partition coefficient,  $K_d$  in Eq. (4-9). 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 the  $\beta$ -SOAR only considers sorption to fixed 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.

Radionuclide-specific sorption coefficients ( $K_d$ ), bulk density ( $\rho_b$ ), effective porosity ( $\theta$ ), 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 porous medium were based on studies of alluvium for the Yucca Mountain project (DOE, 2008).

#### 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, sandstone, or clay. 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.

### 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

$$E = \sum_i m_i \times \frac{CF}{Q} \times a_i \times I \times d_i \times C^* \quad 4-10$$

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  $i$ ,  $C^*$  is the product of unit conversions for volume [acre-ft/L], activity [Bq/Ci], and dose equivalent [mrem/Sv].

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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.

Integrated release is calculated as described in 40 CFR 191, Appendix A, Table 1 for Subpart B. This calculation in β-SOAR assumes that the initial inventory falls into the category of Note 1(a) of Table 1 in 40 CFR 191 Subpart B, 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 consumed by the receptor 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 95<sup>th</sup> 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. Alternative 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).

## 5 MODEL CONFIDENCE

The beta (β) designation in β-SOAR indicates this initial version of the model and the assigned default input parameters are considered preliminary and have yet to undergo rigorous review and validation. A preliminary level of confidence that the model is performing calculations correctly has been attained, however, during the development process through in-progress testing and review of each model component and evaluation of intermediate and total-system results to ensure the individual model elements are reading inputs, performing calculations, and passing outputs to other model elements correctly. A brief summary of the model review and testing conducted to gain model confidence at the time this user guide was prepared is provided in the following bullet list.

- All GoldSim model elements (e.g., data elements, mixing cells, pipe pathways, selectors, results elements, etc.) were visually checked to ensure correct algorithms are implemented, correct units are used, and inputs and outputs flow to the correct elements. For most model elements, text descriptions were added to aid users in understanding the purpose of the element.
- Individual realizations were run using high and low input parameter values and results were compared to ensure the model intermediate and system-level response is correct. For example, for each waste package material, the model was run using highest and lowest waste form degradation rate and results compared to ensure higher waste form degradation rates result 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 ensure the model selects 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 ensure resulting output responded proportionally.
- Hand calculations and spreadsheet calculations were used to check dose calculations in the Biosphere model component at discrete time steps.

Model testing activities are ongoing and are being documented as they are completed. Formal documentation of model testing and benchmarking activities will be prepared to support removal of the beta designation when the model is considered complete.



## 6 RISK INSIGHTS

[This section is reserved until completion of the SOAR model (post beta). Areas of potential additional model development are listed in Appendix C. Insights will be coordinated with the technical findings and priorities identified in the Key Technical and Regulatory Issues document.]

## 7 REFERENCES

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## **APPENDIX A**

### **Default Input Parameters**

**Table A-1. Default Parameters for  $\beta$ -SOAR Waste Form Model Component**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
Initial_Inventory_CSNF	CSNF Radionuclide Inventory (g) [C14, Cs135, I129, Np237, Pu238, Pu239, Pu240, Pu242, 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/RW-0573, Rev. 1 Yucca Mountain Repository SAR, Table 2.3.7-3 page 2.3.7-124 and Scientific Notebook #1036 (WF#-0) Note: See the referenced scientific notebook. Inventories for Pu-241 and Am-241 are added to the initial inventory of Np-237 to account for in-growth
Initial_Inventory_HLW_Glass	HLW Glass Radionuclide Inventory (g) [C14, Cs135, I129, Np237, Pu238, Pu239, Pu240, Pu242, 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]	Scientific Notebook #1036E (WF#-0) Note: The representative inventory for HWL Glass is derived based upon values taken from the DOE/RW-0573, Rev. 1, Yucca Mountain Repository SAR (YM-SAR). Because there is some uncertainty on what the inventory will be for a future glass, a representative bounding glass has been created based upon the YM-SAR, Table 1.5.1-21, pages 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, SRS, West Valley, and Idaho) by selecting the maximum radionuclide inventories from the four types presented in Table 1.5.1-21 of the YM-SAR). Additionally, the inventories for Pu-241 and Am-241 are added to the initial inventory of Np-237 to account for in-growth
Initial_Inventory_sMOX	sMOX Radionuclide Inventory (g) [C14, Cs135, I129, Np237, Pu238, Pu239, Pu240, Pu242, 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]	ANL-WIS-MD-000022 Rev. 01, MOX Spent Nuclear Fuel and LaBS Glass for TSPA-LA, Table 6-2 page 9 and Scientific Notebook #1036E (WF#-0) Note: The inventories for Pu-241 and Am-241 are added to the initial inventory of Np-237 to account for in-growth

**Table A-1. Default Parameters for  $\beta$ -SOAR Waste Form Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
DegRate_CSNF_Oxidizing	CSNF Waste Form Degradation Rate ( $\text{yr}^{-1}$ )	Log-uniform 3.00E-05, 6.00E-04	1. Leslie, B., C. Grossman, and J. Durham. 2007. Total-System Performance Assessment (TPA) Version 5.1 Module Description and User Guide. ML072710060. San Antonio, Texas: CNWRA. 2. Nuclear Regulatory Commission (NRC). 2008. NUREG-1914., Dissolution Kinetics of Commercial Spent Nuclear Fuels in the Potential Yucca Mountain Repository Environment. ML 083120074. Washington, DC: NRC 3. Shoesmith, D. W. 2000. Fuel Corrosion Processes under Waste Disposal Conditions. Journal of Nuclear Materials. Vol. 282. pp. 1-31.
DegRate_CSNF_Reducing	CSNF Waste Form Degradation Rate ( $\text{yr}^{-1}$ )	Log-uniform 9.00E-07, 2.00E-05	1. Leslie, B., C. Grossman, and J. Durham. 2007. Total-System Performance Assessment (TPA) Version 5.1 Module Description and User Guide. ML072710060. San Antonio, Texas: CNWRA. 2. Nuclear Regulatory Commission (NRC). 2008. NUREG-1914., Dissolution Kinetics of Commercial Spent Nuclear Fuels in the Potential Yucca Mountain Repository Environment. ML 083120074. Washington, DC: NRC 3. Shoesmith, D. W. 2000. Fuel Corrosion Processes under Waste Disposal Conditions. Journal of Nuclear Materials. Vol. 282. pp. 1-31.
DegRate_CSNF_Combined	CSNF Waste Form Degradation Rate ( $\text{yr}^{-1}$ )	Log-uniform 9.00E-07, 6.00E-04	1. Leslie, B., C. Grossman, and J. Durham. 2007. Total-System Performance Assessment (TPA) Version 5.1 Module Description and User Guide. ML072710060. San Antonio, Texas: CNWRA. 2. Nuclear Regulatory Commission (NRC). 2008. NUREG-1914., Dissolution Kinetics of Commercial Spent Nuclear Fuels in the Potential Yucca Mountain Repository Environment. ML 083120074. Washington, DC: NRC 3. Shoesmith, D. W. 2000. Fuel Corrosion Processes under Waste Disposal Conditions. Journal of Nuclear Materials. Vol. 282. pp. 1-31.

**Table A-1. Default Parameters for  $\beta$ -SOAR Waste Form Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
DegRate_sMOX_Oxidizing	sMOX Waste Form Degradation Rate ( $\text{yr}^{-1}$ )	Log-uniform 3.00E-05, 6.00E-04	1. Ebert, W. L., M. A. Lewis, T. L. Barber, and S. G. Johnson, 2002. "Accounting for EBR-II Metallic Waste Form Degradation in TSPA." Scientific Basis for Nuclear Waste Management XXVI. R. J. Finch and D. B. Bullen (eds.) Materials Research Society Symposium Proceedings. Vol. 757. Warrendale, Pennsylvania: Materials Research Society. pp. 71–80. 2. Wang, Y. 2009. "Adaptive Waste Forms: The Concept and Its Implications." Presentation at Integrated Radioactive Waste Management in Future Fuel Cycles, November 8 – 12, 2009, Charleston, South Carolina, USA
DegRate_sMOX_Reducing	sMOX Waste Form Degradation Rate ( $\text{yr}^{-1}$ )	Log-uniform 9.00E-07, 2.00E-05	1. Ebert, W. L., M. A. Lewis, T. L. Barber, and S. G. Johnson, 2002. "Accounting for EBR-II Metallic Waste Form Degradation in TSPA." Scientific Basis for Nuclear Waste Management XXVI. R. J. Finch and D. B. Bullen (eds.) Materials Research Society Symposium Proceedings. Vol. 757. Warrendale, Pennsylvania: Materials Research Society. pp. 71–80. 2. Wang, Y. 2009. "Adaptive Waste Forms: The Concept and Its Implications." Presentation at Integrated Radioactive Waste Management in Future Fuel Cycles, November 8 – 12, 2009, Charleston, South Carolina, USA
DegRate_sMOX_Combined	sMOX Waste Form Degradation Rate ( $\text{yr}^{-1}$ )	Log-uniform 9.00E-07, 6.00E-04	1. Ebert, W. L., M. A. Lewis, T. L. Barber, and S.G. Johnson, 2002. "Accounting for EBR-II Metallic Waste Form Degradation in TSPA." Scientific Basis for Nuclear Waste Management XXVI. R. J. Finch and D. B. Bullen (eds.) Materials Research Society Symposium Proceedings. Vol. 757. Warrendale, Pennsylvania: Materials Research Society. pp. 71–80. 2. Wang, Y. 2009. "Adaptive Waste Forms: The Concept and Its Implications." Presentation at Integrated Radioactive Waste Management in Future Fuel Cycles, November 8 – 12, 2009, Charleston, South Carolina, USA

**Table A-1. Default Parameters for  $\beta$ -SOAR Waste Form Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
DegRate_HLW_Glass	HLW Glass Waste Form Degradation Rate ( $\text{yr}^{-1}$ )	Log-uniform 1.50E-06, 2.00E-04	1. Bechtel SAIC Company. 2004. Defense HLW Glass Degradation Model. ANL-EBS-MD-000016. Rev. 02. ACN 001., ERD 001, ERD, 002. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2. Van Iseghem, P. 2007. "Geological Disposal of Radioactive Waste – the Challenge of Assessing the Long-term Safety." Mol, Belgium: SCK.CEN
UnboundFraction_CSNF_Cs135	Cs135 Unbound fraction for CSNF (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0088, 0.025, 0.058	NRC-02-02-012: Total-System Performance Assessment (TPA) Version 5.1 Module Descriptions and User Guide 08/2007, from Table 10-1 pages 10-43 and 10-44 / Scientific Notebook #1036E
UnboundFraction_CSNF_I129	I129 Unbound fraction for CSNF (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0054, 0.11, 0.32	NRC-02-02-012: Total-System Performance Assessment (TPA) Version 5.1 Module Descriptions and User Guide 08/2007, from Table 10-1 pages 10-43 and 10-44 / Scientific Notebook #1036E
UnboundFraction_CSNF_Tc99	Tc99 Unbound fraction for CSNF (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0005, 0.0013, 0.0028	NRC-02-02-012: Total-System Performance Assessment (TPA) Version 5.1 Module Descriptions and User Guide 08/2007, from Table 10-1 pages 10-43 and 10-44 / Scientific Notebook #1036E
UnboundFraction_CSNF_C14	C14 Unbound fraction for CSNF (Instant Release Fraction from GAP/grain inventory)	Discrete 1, 0.1	ML043020321 V. Jain, G. Cragnolino, L. Howard, A Review Report on High Burnup Spent Nuclear Fuel-Disposal Issues, Table 4-3 page 4-11 / Scientific Notebook #1036E
UnboundFraction_MOX_Cs135	Cs135 Unbound fraction for MOX (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0088, 0.025, 0.058	NRC-02-02-012: Total-System Performance Assessment (TPA) Version 5.1 Module Descriptions and User Guide 08/2007, from Table 10-1 pages 10-43 and 10-44 / Scientific Notebook #1036E
UnboundFraction_MOX_I129	I129 Unbound fraction for MOX (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0054, 0.11, 0.32	NRC-02-02-012: Total-System Performance Assessment (TPA) Version 5.1 Module Descriptions and User Guide 08/2007, from Table 10-1 pages 10-43 and 10-44 / Scientific Notebook #1036E
UnboundFraction_MOX_Tc99	Tc99 Unbound fraction for MOX (Instant Release Fraction from GAP/grain inventory)	Triangular 0.0005, 0.0013, 0.0028	NRC-02-02-012: Total-System Performance Assessment (TPA) Version 5.1 Module Descriptions and User Guide 08/2007, from Table 10-1 pages 10-43 and 10-44 / Scientific Notebook #1036E



**Table A-1. Default Parameters for  $\beta$ -SOAR Waste Form Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
UnboundFraction_MOX_C14	C14 Unbound fraction for MOX (Instant Release Fraction from GAP/grain inventory)	Discrete 1, 0.1	ML043020321 V.Jain, G. Cragnolino, L. Howard, A Review Report on High Burnup Spent Nuclear Fuel-Disposal Issues, Table 4-3 page 4-11 / Scientific Notebook #1036E
Ea_SF	Activation energy for spent fuel (J/mol)	Discrete 1, 34300	Leslie, B., C. Grossman, and J. Durham. 2007. Total-System Performance Assessment (TPA) Version 5.1 Module Description and User Guide. ML072710060. San Antonio, Texas: CNWRA.
Ea_Glass	Activation energy for glass (J/mol)	Discrete 1, 40000	DOE RAI 3.2.2.1.1-005 Table 1.1-2
Ea_sMOX	Activation energy for sMOX (J/mol)	Discrete 1, 34300	1. Ebert, W. L., M. A. Lewis, T. L. Barber, and S. G. Johnson, 2002. "Accounting for EBR-II Metallic Waste Form Degradation in TSPA." Scientific Basis for Nuclear Waste Management XXVI. R. J. Finch and D. B. Bullen (eds.) Materials Research Society Symposium Proceedings. Vol. 757. Warrendale, Pennsylvania: Materials Research Society. pp. 71–80. 2. Wang, Y. 2009. "Adaptive Waste Forms: The Concept and Its Implications." Presentation at Integrated Radioactive Waste Management in Future Fuel Cycles, November 8–12, 2009, Charleston, South Carolina, USA
ModDegRate_CSNF_Distribution	Factor to adjust the degradation rate for CSNF	Discrete 1, 1	Flexibility parameter; only used if dashboard value of Degradation Rate Multiplier for CSNF is set to zero
ModDegRate_HLW_Distribution	Factor to adjust the degradation rate for HLW	Discrete 1, 1	Flexibility parameter; only used if dashboard value of Degradation Rate Multiplier for HLW is set to zero
ModDegRate_sMOX_Distribution	Factor to adjust the degradation rate for sMOX	Discrete 1, 1	Flexibility parameter; only used if dashboard value of Degradation Rate Multiplier for sMOX is set to zero
Releasable_CSNF_Distribution	Fraction of the inventory that could be released after WP failure	Discrete 1, 1	Flexibility parameter; only used if dashboard value of Fraction of WF Inventories Available for Release is set to zero for CSNF
Releasable_HLW_Distribution	Fraction of the inventory that could be released after WP failure	Discrete 1, 1	Flexibility parameter; only used if dashboard value of Fraction of WF Inventories Available for Release is set to zero for HLW

Table A-1. Default Parameters for $\beta$ -SOAR Waste Form Model Component (continued)			
Parameter Name	Description	Distribution Type & Values	Reference/Rationale
Releasable_sMOX_Distribution	Fraction of the inventory that could be released after WP failure	Discrete 1, 1	Flexibility parameter; only used if dashboard value of Fraction of WF Inventories Available for Release is set to zero for sMOX

Table A-2. Default Parameters for $\beta$ -SOAR Waste Package Model Component			
Parameter Name	Description	Distribution Type & Values	Reference/Rationale
WP_Number	Number of Waste Packages	Constant 10000	MDL-WIS-PA-000005 REV00: Total-System Performance Assessment Model/Analysis for the License Application.
WP_Thickness_CS	Carbon Steel WP Thickness (cm)	Constant 10	International countries reported 3-25 cm as the carbon steel container thickness. The rounded average value of 10 cm is chosen for beta SOAR.
WP_Thickness_Cu	Copper WP Thickness (cm)	Constant 2.5	Canada proposes 2.5 cm and both Finland and Sweden proposes 5 cm, based on Table 1-1 from Kursten, B., E. Smailos, I. Azkarate, L. Werme, N.R. Smart, G. Santarini. "State-of-the-art Document on the Corrosion Behavior of Container Materials." European Commission. 2004. The thinnest value of 2.5 cm was chosen as the container thickness in beta SOAR.
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; Germany proposes 3-4 mm; YM drip shield thickness is 15 mm; no thickness data is available from Japan although Ti is proposed (COBECOMA report by Kursten et al., 2004, Table 1-1. Select 10 mm as the thickness, which is near the average of all available data.
WP_Surface	Surface of the waste package, used to define cross sections for advective and diffusive release from the WP (m <sup>2</sup> )	Constant 40	Based on YM project design.
Cu_GC_Ox_Low	Copper, low bound for the corrosion rate, oxidizing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 0.04	Based on Swedish data reported in Paul Wersin, Kastriot Spahiu and Jordi Bruno. 1994. Kinetic modeling of bentonite-canister interaction Long-term predictions of copper canister corrosion under oxic and anoxic conditions. SKB TR 94-25. MBT Tecnología Ambiental, Cerdanyola, Spain, September 1994. A pitting enhancement factor of 5 was considered. If sulfate concentration could be higher than what used in the Swedish report, another enhancement factor should be considered. Log-normal distribution is used.

**Table A-2. Default Parameters for  $\beta$ -SOAR Waste Package Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
Cu_GC_Ox_High	Copper, high bound for the corrosion rate, oxidizing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 7	Based on Swedish data reported in Paul Wersin, Kastriot Spahiu and Jordi Bruno. 1994. Kinetic modeling of bentonite-canister interaction Long-term predictions of copper canister corrosion under oxic and anoxic conditions. SKB TR 94-25. MBT Tecnología Ambiental, Cerdanyola, Spain, September 1994. 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.
Cu_GC_Anox_Low	Copper, low bound for the corrosion rate, reducing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 0.004	Based on Swedish data reported in Paul Wersin, Kastriot Spahiu and Jordi Bruno. 1994. Kinetic modeling of bentonite-canister interaction Long-term predictions of copper canister corrosion under oxic and anoxic conditions. SKB TR 94-25. MBT Tecnología Ambiental, Cerdanyola, Spain, September 1994. A pitting enhancement factor of 5 was considered. If sulfate concentration could be higher than what used in the Swedish report, another enhancement factor should be considered. Log-normal distribution is used.
Cu_GC_Anox_High	Copper, high bound for the corrosion rate, reducing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 0.02	Based on Swedish data reported in Paul Wersin, Kastriot Spahiu and Jordi Bruno. 1994. Kinetic modeling of bentonite-canister interaction Long-term predictions of copper canister corrosion under oxic and anoxic conditions. SKB TR 94-25. MBT Tecnología Ambiental, Cerdanyola, Spain, September 1994. A pitting enhancement factor of 5 was considered. Uncertainty remains on sulfate concentration. If sulfate concentration could be higher than what used in the Swedish report, another enhancement factor should be considered. Log-normal distribution is used.
CS_GC_Ox_Low	Carbon Steel, low bound for the corrosion rate, oxidizing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 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. The distribution is log-uniform in oxidizing condition. References are: [J. of Nuclear Materials (JNM), 379, 2008, Proceedings of the Third International Workshop on Long-Term Prediction of Corrosion Damage in Nuclear Waste Systems, University Park, PA, May 14-18, 2007. Vol. 3; D. G. Bennett and R. Gens, Overview of European Concepts for High-Level Waste and Spent Fuel Disposal with Special Reference Waste Container Corrosion,

**Table A-2. Default Parameters for  $\beta$ -SOAR Waste Package Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			<p>pp 1–8; L. Johnson and F. King, The effect of the Evolution of Environmental Conditions on the Corrosion Evolutionary Path in a Repository for Spent Fuel and High-Level Waste in Opalinus Clay, pp 9–5, and; D. Feron, D. Crusset and J.-M. Gras, Corrosion Issues in Nuclear Waste Disposal, pp. 16–23]</p> <p>[T. Ahn and P. Soo, Corrosion of Low-Carbon Cast Steel in Concentrated Synthetic Groundwater at 80 to 150 EC, Waste Management, 15, 1995, pp 471–476; related T. Ahn and B. Leslie, Corrosion Products of Steels in High-Level Waste Management at the Proposed Yucca Mountain Repository, 1998, NUDOC 9808060163, ADAMS ML031671314]</p> <p>[Prediction of Long Term Corrosion Behavior in Nuclear Waste Systems, Proceedings of the 2nd International Workshop, European Federation of Corrosion, Nice, September 2004, Eurocorr, 2004. Vol. 2; N. Taniguchi, M. Kawasaki, S. Kawakami and M. Kubota, Corrosion Behavior of Carbon Steel in Contact with Bentonite under Anaerobic Conditions, pp. 24–34.</p> <p>F. Foct, J. Cabrea, W. Dridi and S. Savoye, Corrosion behavior of Carbon Steel in the Tounemire Clay, pp. 68–77, and; B. Kursten, E. Smailos, I. Azarate, L. Wermer, N. R. Smart, G. Marx, M. A. Cunado and G. Santarini, Corrosion Evaluation of Metallic HLW/ Spent Fuel Disposal Containers – Review, pp. 153–161]</p> <p>[European Federation of Corrosion Publications, Number 36 Prediction of Long Term Corrosion Behavior in Nuclear Waste Systems, ed. By D. Feron and D. Macdonald, The European Federation of Corrosion on behalf of the Institute of Materials, Minerals and Mining, Vol. 1</p> <p>F. Foct and J.-M. Gras, Semi-Empirical Model for Carbon Steel Corrosion in Long Term Geological Nuclear Waste Disposal, pp. 91–102]</p> <p>[European Commission, State-of-the-Art Document on the Corrosion Behavior of Container Materials, B. Kursten et al., 2004]</p> <p>[MRS Proceedings on Scientific Basis for Nuclear Waste Management]</p>
CS_GC_Ox_High	Carbon Steel, high bound for the corrosion rate, oxidizing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 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. The distribution is log-uniform in oxidizing condition. References are the same as above.

**Table A-2. Default Parameters for  $\beta$ -SOAR Waste Package Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
CS_GC_Annox_Low	Carbon Steel, low bound for the corrosion rate, reducing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 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. The distribution is log-normal in reducing condition. References are the same as above.
CS_GC_Annox_High	Carbon Steel, high bound for the corrosion rate, reducing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 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. The distribution is log-normal in reducing condition. References are the same as above.
SS_GC_Ox_Low	Stainless Steel, low bound for the corrosion rate, oxidizing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 0.01	Select Switch_GC_DistributionType=1(normal), Switch_GC_DistributionScale=1(log); i.e., log-normal distribution in corrosion rates. Based on the minimum corrosion rate from YMP project in-package condition for stainless steel (BSC, 2007).Reference: BSC. 2007. EBS Radionuclide Transport Abstraction. Table 4.1-1. ANL-WIS-PA-000001 REV 03.
SS_GC_Ox_High	Stainless Steel, high bound for the corrosion rate, oxidizing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 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 report by Kursten et al. (2003), Table 4-54 and Figure 4-72. Tests were conducted at pH of 1.9-13 and temperatures of 30-80°C. The corrosion rate increased with decreasing pH. At pH of 4 and 80 °C, the corrosion rate was 2.6 $\mu\text{m}/\text{yr}$ . Based on other data from international geological repository program, 3 $\mu\text{m}/\text{yr}$ 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, 2004). A distribution type skewing towards lower end is reasonable.
SS_GC_Annox_Low	Stainless Steel, low bound for the corrosion rate, reducing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 0.003	Based on Kursten et al. (2003), Table 4-34. This low rate is also near the resolution limit of the weight loss analysis method to determine corrosion rate.
SS_GC_Annox_High	Stainless Steel, high bound for the corrosion rate, reducing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 0.1	Based on corrosion studies performed in cementitious backfill material, Kursten et al. (2003) summarized that the long-term anoxic corrosion rate of stainless steel at all repository temperatures is <0.01 $\mu\text{m}/\text{yr}$ . Based on <i>in-situ</i> corrosion studies relevant to the Belgian disposal concept in clay, Kursten et al. (2003) summarized that the maximum corrosion rate was 0.15 $\mu\text{m}/\text{yr}$ at 170 °C with most of the corrosion rates less than 0.1 $\mu\text{m}/\text{yr}$ . Based on these limited data in anoxic condition, it is

**Table A-2. Default Parameters for  $\beta$ -SOAR Waste Package Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			reasonable to assume that the maximum corrosion rate is 0.1 $\mu$ m/yr. A distribution skewing towards the lower end is preferred.
Ti_GC_Ox_Low	Titanium, low bound for the corrosion rate, oxidizing medium ( $\mu$ m/yr)	Discrete 1, 0.008	The general corrosion rates are based on literature review of corrosion rates in possible repository conditions from international countries who 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 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. Log-normal distribution in corrosion rates.
Ti_GC_Ox_High	Titanium, high bound for the corrosion rate, oxidizing medium ( $\mu$ m/yr)	Discrete 1, 0.2	The general corrosion rates are based on literature review of corrosion rates in possible repository conditions from international countries who 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 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. Log-normal distribution in corrosion rates.
Ti_GC_Anox_Low	Titanium, low bound for the corrosion rate, reducing medium ( $\mu$ m/yr)	Discrete 1, 0.008	The general corrosion rates are based on literature review of corrosion rates in possible repository conditions from international countries who 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

**Table A-2. Default Parameters for  $\beta$ -SOAR Waste Package Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			media because 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. Log-normal distribution in corrosion rates.
Ti_GC_Annox_High	Titanium, high bound for the corrosion rate, reducing medium ( $\mu\text{m}/\text{yr}$ )	Discrete 1, 0.2	The general corrosion rates are based on literature review of corrosion rates in possible repository conditions from international countries who 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 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. log-normal distribution in corrosion rates.
LC_FailureTime_Period_I	Failure time by LC for the early Period I (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 (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. (Taniguchi, N., M. Kawasaki, S. Kawakami, M. Kubota. "Corrosion Behavior of Carbon Steel in Contact with Bentonite under Anaerobic Condition. Proceedings of the 2nd International Prediction of Long Term Corrosion Behavior in Nuclear Waste Systems Workshop. 2004.) Wersin et al. (1994) reported a maximum period of 280 years for oxidizing condition (Paul Wersin, Kastriot Spahiu and Jordi Bruno. 1994. Kinetic modeling of



**Table A-2. Default Parameters for  $\beta$ -SOAR Waste Package Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			bentonite-canister interaction Long-term predictions of copper canister corrosion under oxic and anoxic conditions. SKB TR 94-25. MBT Tecnología Ambiental, Cerdanyola, Spain, September 1994.). WP Workshop Vol. 1, p. 101 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
LC_FailureTime_Period_I	Failure time by LC for the late Period II (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.
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 <u>reducing media</u> . 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 1000 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 (0.5X0.5). A triangular distribution is used to have the most likely value in the middle.
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 higher chance to exhibit 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.
X_Prob_LC_Period_I	Fraction of waste packages failed by LC during the early Period I (X=Cu, CS, Ti) (unitless)	Constant 0	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. This probability parameter is used for all materials except stainless steel (the stainless steel probability is defined in separate parameters). A probability equal to 0 was selected for all of the other materials than stainless steel: titanium localized corrosion is not considered, and pitting corrosion of carbon steel and copper is considered by multiplying an enhancement factor to the general corrosion rate.

**Table A-2. Default Parameters for  $\beta$ -SOAR Waste Package Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
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 <u>reducing media</u> . 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.
SS_Prob_LC_Period_II_Oxidizing	Fraction of SS waste packages failed by LC during the late Period II in oxidizing environment (unitless)	Discrete 1, 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.
X_Prob_LC_Period_II	Fraction of waste packages failed by LC during the late Period II (X=Cu, CS, Ti) (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. This probability parameter is used for all materials except stainless steel (the stainless steel probability is defined in separate parameters). A probability equal to 0 was selected for all of the other materials than stainless steel: titanium localized corrosion is not considered, and pitting corrosion of carbon steel and copper is considered by multiplying an enhancement factor to the general corrosion rate.
GC_FractionAreaBreached	Fraction of WP area breached by general corrosion (unitless)	Discrete 1, 1	No credit is taken for damage area due to general corrosion since general corrosion is wide-spread.
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 to form crevice 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 due to the fact that 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 considered. A log-triangular distribution is considered.

**Table A-3. Default Parameters for  $\beta$ -SOAR Near Field Model Component**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
Backfill_ExpectedLifetime	Average lifetime of backfill material (yr)	Discrete 1, 1.00E+06	Requires further analysis. Base case will assume no cracking failure of backfill. Value should therefore be greater than simulation period.
Backfill_InitialFailureTime	Time at which backfill units start failing (yr)	Discrete 1, 1.00E+06	Requires further analysis. Base case will assume no cracking failure of backfill. Value should therefore be greater than simulation period.
Backfill_FractionCracked	Fraction of a backfill unit covered by cracks after failure occurs (unitless)	Discrete 1,0	Flexibility parameter. Base case will assume no cracking failure of backfill.
Backfill_Porosity	Initial porosity of the backfill unit (unitless)	Discrete 1, 0.44	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-8. Treated as constant for this model because variability is small compared to uncertainty in Kd values.
Backfill_SpecificDensity	Backfill specific density (kg/m <sup>3</sup> )	Discrete 1, 2000	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-8. Treated as constant for this model because variability is small compared to uncertainty in Kd values
Dc_Cs_Free	Diffusivity of Cs in free water (m <sup>2</sup> /s)	Discrete 1, 2.10E-09	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Svensk Kärnbränslehantering AB. November 2006 Stockholm Sweden: Swedish Nuclear Fuel and Waste Management Co., p. 242, Table A-40 (Recommended value for diffusivities in free solution /Ohlsson and Neretnieks 1997.) The recommended diffusion coefficients in free solution are of the order of 1E-9 m <sup>2</sup> /s, which are consistent with diffusion coefficients of electrolytes and non-electrolytes in the Handbook of Chemistry and Physics at 25 °C.
Dc_I_Free	Diffusivity of I in free water (m <sup>2</sup> /s)	Discrete 1, 8.30E-10	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Svensk Kärnbränslehantering AB. November 2006 Stockholm Sweden: Swedish Nuclear Fuel and Waste Management Co., p. 242, Table A-40 (Recommended value for diffusivities in free solution /Ohlsson and Neretnieks 1997.) The recommended diffusion coefficients in free solution are of the order of 1E-9 m <sup>2</sup> /s, which are consistent with diffusion coefficients of electrolytes and non-electrolytes in the Handbook of Chemistry and Physics at 25 °C.

**Table A-3. Default Parameters for  $\beta$ -SOAR Near Field Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
Dc_Np_Free	Diffusivity of Np in free water (m <sup>2</sup> /s)	Discrete 1, 1.00E-09	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Svensk Kärnbränslehantering AB. November 2006. Stockholm Sweden: Swedish Nuclear Fuel and Waste Management Co., p. 242, Table A-40 (Recommended value for diffusivities in free solution /Ohlsson and Neretnieks 1997.) The recommended diffusion coefficients in free solution are of the order of 1E-9 m <sup>2</sup> /s, which are consistent with diffusion coefficients of electrolytes and non-electrolytes in the Handbook of Chemistry and Physics at 25 °C.
Dc_Pu_Free	Diffusivity of Pu in free water (m <sup>2</sup> /s)	Discrete 1, 1.00E-09	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Svensk Kärnbränslehantering AB. November 2006 Stockholm Sweden: Swedish Nuclear Fuel and Waste Management Co., p. 242, Table A-40 (Recommended value for diffusivities in free solution /Ohlsson and Neretnieks 1997.) The recommended diffusion coefficients in free solution are of the order of 1E-9 m <sup>2</sup> /s, which are consistent with diffusion coefficients of electrolytes and non-electrolytes in the Handbook of Chemistry and Physics at 25 °C.
Dc_Tc_Free	Diffusivity of Tc in free water (m <sup>2</sup> /s)	Discrete 1, 1.00E-09	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Svensk Kärnbränslehantering AB. November 2006 Stockholm Sweden: Swedish Nuclear Fuel and Waste Management Co., p. 242, Table A-40 (Recommended value for diffusivities in free solution /Ohlsson and Neretnieks 1997.) The recommended diffusion coefficients in free solution are of the order of 1E-9 m <sup>2</sup> /s, which are consistent with diffusion coefficients of electrolytes and non-electrolytes in the Handbook of Chemistry and Physics at 25 °C.
Dc_U_Free	Diffusivity of U in free water (m <sup>2</sup> /s)	Discrete 1, 1.00E-09	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Svensk Kärnbränslehantering AB. November 2006

**Table A-3. Default Parameters for  $\beta$ -SOAR Near Field Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			Stockholm Sweden: Swedish Nuclear Fuel and Waste Management Co., p. 242, Table A-40 (Recommended value for diffusivities in free solution /Ohlsson and Neretnieks 1997.) The recommended diffusion coefficients in free solution are of the order of 1E-9 m <sup>2</sup> /s, which are consistent with diffusion coefficients of electrolytes and non-electrolytes in the Handbook of Chemistry and Physics at 25 °C.
Dc_C_Free	Diffusivity of C in free water (m <sup>2</sup> /s)	Discrete 1, 1.20E-09	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Svensk Kärnbränslehantering AB. November 2006. Stockholm Sweden: Swedish Nuclear Fuel and Waste Management Co. p. 242, Table A-40. Recommended diffusion coefficients in free solution are of the order of 1E-9 m <sup>2</sup> /s, consistent with diffusion coefficients of electrolytes and non-electrolytes in the Handbook of Chemistry and Physics at 25 °C.
Dc-Cs_Backfill	Diffusivity of Cs in backfill material (m <sup>2</sup> /s)	Uniform 4.94E-11, 1.91E-10	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-11. Uniform distribution selected to equally weight full range of uncertainty.
Dc-I_Backfill	Diffusivity of I in backfill material (m <sup>2</sup> /s)	Uniform 3.0E-12, 3.0E-11	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. 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-Np_Backfill	Diffusivity of Np in backfill material (m <sup>2</sup> /s)	Uniform 4.94E-11, 1.91E-10	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-11. Uniform distribution selected to equally weight full range of uncertainty.
Dc-Pu_Backfill	Diffusivity of Pu in backfill material (m <sup>2</sup> /s)	Uniform 4.94E-11, 1.91E-10	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-11. Uniform distribution selected to equally weight full range of uncertainty.
Dc-Tc_Backfill	Diffusivity of Tc in backfill material (m <sup>2</sup> /s)	Uniform 4.94E-11, 1.91E-10	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-11. Uniform distribution selected to equally weight full range of uncertainty.
Dc-U_Backfill	Diffusivity of U in backfill material (m <sup>2</sup> /s)	Uniform 4.94E-11, 1.91E-10	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-11. Uniform distribution selected to equally weight full range of uncertainty.
Dc-C_Backfill	Diffusivity of C in backfill material (m <sup>2</sup> /s)	Uniform 3.0E-12, 3.0E-11	SKB, 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-11. Uniform distribution

**Table A-3. Default Parameters for  $\beta$ -SOAR Near Field Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			selected to equally weight full range of uncertainty. Note that range of values for is smaller because carbonate species and organic acids are subject to anion exclusion.
Dc_Ea	Activation energy for the diffusion coefficient (J/mol)	Discrete 1, 1.51E+04	Japan Nuclear Cycle Development Institute (JNC). 2000. "H12: Project to Establish the Scientific and Technical Basis for HLW Disposal in Japan, Supporting Report 3, Safety Assessment of the Geological Disposal System." JNC TN 1410 2000-004. Japan: Japan Nuclear Cycle Development Institute. p. V-43
Solubility_Cs_Ox	Cs solubility in backfill, oxidizing conditions (mg/L)	Discrete 1, -1	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98 . 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_I_Ox	I solubility in backfill, oxidizing conditions (mg/L)	Discrete 1, -1	No reference available for Iodide solubility in oxidizing waters. Based on SKB Technical report TR-06-32 indicates no solubility limit for Cs and Tc, it seems reasonable to assume the same for iodide.
Solubility_Np_Ox	Np solubility in backfill, oxidizing conditions (mg/L)	Log-uniform 8.00E-01, 8.00E+01	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98 . Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm, indicating 1.7E-5 mol/L Np2O5, which translates to 8 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. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98 . 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_Tc_Ox	Tc solubility in backfill, oxidizing conditions (mg/L)	Discrete 1, -1	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98. Value for oxidizing conditions is based on the table column for pco2 = 0.2 atm.

**Table A-3. Default Parameters for  $\beta$ -SOAR Near Field Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
Solubility_U_Ox	U solubility in backfill, oxidizing conditions (mg/L)	Log-Uniform 4.50E-01, 4.50E+01	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98. Value for oxidizing conditions is based on the table column for $p_{CO_2} = 0.2$ atm which indicates $1.7 \times 10^{-6}$ mol/L as uranophane plus $2.5 \times 10^{-6}$ mol/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_C_Ox	C solubility in backfill, oxidizing conditions (mg/L)	Log-Uniform 8, 8.50E+02	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98. Value for oxidizing conditions is based on the table column for $p_{CO_2} = 0.2$ atm, indicating a value of $7.1 \times 10^{-3}$ 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-Cs_Red	Cs solubility in backfill, reducing conditions (mg/L)	Discrete 1, -1	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98. 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_Red	I solubility in backfill, reducing conditions (mg/L)	Discrete 1, -1	No reference available for Iodide solubility. Base case assumes no solubility limit.
Solubility_Np_Red	Np solubility in backfill, reducing conditions (mg/L)	Log-Uniform 2.6E-05, 2.6E-03	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98. Value for reducing conditions is based on the table column for bentonite, indicating $1.1 \times 10^{-9}$ mol/L $NpO_2$ , which translates to $2.6 \times 10^{-4}$ mg/L. To consider uncertainty, the range given evaluates approximately one order of magnitude above and below.
Solubility_Pu_Red	Pu solubility in backfill, reducing conditions (mg/L)	Log-Uniform 3.0E-01, 3.0E+01	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98. Value for reducing conditions is based on the table column for bentonite, indicating $1.3 \times 10^{-5}$ mol/L of dominant phase $PuOHCO_3$ . This translates to about 3 mg/L. To

**Table A-3. Default Parameters for  $\beta$ -SOAR Near Field Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			consider uncertainty, the range given evaluates approximately one order of magnitude above and below this value.
Solubility_Tc_Red	Tc solubility in backfill, reducing conditions (mg/L)	Log-Uniform 4.0E-05, 4.0E-03	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98 . Value for reducing conditions is based on the table column for bentonite, indicating 4.4e-9 mo/L of dominant phase TcO <sub>2</sub> . 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_Red	U solubility in backfill, reducing conditions (mg/L)	Log-Uniform 3.00E-01, 3.00E+01	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98 . 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.
Solubility_C_Red	C solubility in backfill, reducing conditions (mg/L)	Log-Uniform 4.8, 4.80E+02	SKB. 2006. Determination and assessment of the concentration limits to be used in SR-Can. Technical Report TR-06-32. Table 8-1 on pp. 97-98 . Value for reducing conditions is based on the table column for bentonite, indicating a value of 3.99e-3 mol/L for CaCO <sub>3</sub> 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_Ea	Activation energy for solubility (J/mol)	Discrete 1, 6.00E+03	Need Reference
Kd_Cs_BF_Ox	Kd of Cs in backfill material, oxidizing conditions (m <sup>3</sup> /kg)	Log-Uniform 0.018, 0.6	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 provides range of minimum to maximum recommended values for bentonite buffer. Loguniform distribution is also recommended.
Kd_I_BF_Ox	Kd of I in backfill material, oxidizing conditions (m <sup>3</sup> /kg)	Discrete 1, 0	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 gives zero value for nonsorbing Iodine.
Kd_Np_BF_Ox	Kd of Np in backfill material, oxidizing conditions (m <sup>3</sup> /kg)	Log-Uniform 0.004, 0.2	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 provides range of minimum to maximum recommended values for bentonite buffer.



**Table A-3. Default Parameters for  $\beta$ -SOAR Near Field Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			Loguniform distribution is also recommended. For oxidizing conditions Np(V) is assumed.
Kd_Pu_BF_Ox	Kd of Pu in backfill material, oxidizing conditions ( $\text{m}^3/\text{kg}$ )	Log-Uniform 0.002, 28	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 provides range of minimum to maximum recommended values for bentonite buffer. Loguniform distribution is also recommended. For oxidizing conditions range for both Pu(V) and Pu(VI) are included.
Kd_Tc_BF_Ox	Kd of Tc in backfill material, oxidizing conditions ( $\text{m}^3/\text{kg}$ )	Discrete 1, 0	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 gives zero value for Tc(VII), which is assumed for oxidizing conditions.
Kd_U_BF_Ox	Kd of U in backfill material, oxidizing conditions ( $\text{m}^3/\text{kg}$ )	Log-Uniform 0.5, 18	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 provides range of minimum to maximum recommended values for bentonite buffer. Loguniform distribution is also recommended. For oxidizing conditions range for U(VI) is assumed.
Kd_C_BF_Ox	Kd of C in backfill material, oxidizing conditions ( $\text{m}^3/\text{kg}$ )	Discrete 1, 0	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 gives zero value for nonsorbing carbon.
Kd-Cs_BF_Anox	Kd of Cs in backfill material, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-Uniform 0.018, 0.6	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 provides range of minimum to maximum recommended values for bentonite buffer. Loguniform distribution is also recommended.
Kd_I_BF_Anox	Kd of I in backfill material, reducing conditions ( $\text{m}^3/\text{kg}$ )	Discrete 1, 0	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 gives zero value for nonsorbing iodine.
Kd_Np_BF_Anox	Kd of Np in backfill material, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-Uniform 4, 1113	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 provides range of minimum to maximum recommended values for bentonite buffer. Loguniform distribution is also recommended. For reducing conditions Np(IV) is assumed.
Kd_Pu_BF_Anox	Kd of Pu in backfill material, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-Uniform 4, 1111	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 provides range of minimum to maximum recommended values for bentonite buffer. Loguniform distribution is also recommended. For reducing conditions range for both Pu(III) and Pu(IV) are included.
Kd_Tc_BF_Anox	Kd of Tc in backfill material, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-Uniform 2.3, 1764	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 provides range of

**Table A-3. Default Parameters for  $\beta$ -SOAR Near Field Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			minimum to maximum recommended values for bentonite buffer. Loguniform distribution is also recommended. For reducing conditions Tc(IV) is assumed.
Kd_U_BF_Anox	Kd of U in backfill material, reducing conditions (m <sup>3</sup> /kg)	Log-Uniform 3.6, 1113	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 provides range of minimum to maximum recommended values for bentonite buffer. Loguniform distribution is also recommended. For reducing conditions range for U(IV) is assumed.
Kd_C_BF_Anox	Kd of C in backfill material, reducing conditions (m <sup>3</sup> /kg)	Discrete 1, 0	SKB. 2006. Data report for the safety assessment SR-Can, Technical Report TR-06-25. Table A-12 gives zero value for nonsorbing Carbon.
NF_flowFactor	Factor to adjust the volumetric flux through the near-field, using the far-field volumetric flux as reference (unitless)	Discrete 1, 1	Flexibility parameter
NF_Length	Length of the backfill material used to define the length of diffusive path (m)	Constant 2	Flexibility parameter
NF_Width	Width of the backfill material used to compute cross section for diffusion (m)	Constant 1	Flexibility parameter
NF_Height	Height of the backfill material used to compute cross section for diffusion (m)	Constant 1	Flexibility parameter
f_DiffLengthToFracture	Fraction to compute the effective diffusive distance to the nearest fracture (unitless)	Uniform 0.1, 0.2	Scientific notebook - S. Stothoff
EndThermalPeriod	End of the thermal period, defined as the time for the T to drop to a value equal to (1+q)Tambient (yr)	Uniform 1000, 4000	Not used in this version
q_EndThermalPeriod	q (0<q) factor used to define the end of the thermal period	Constant 0.2	Not used in this version
TemperatureMax	Maximum system temperature (deg. Celsius)	Uniform 90, 100	Not used in this version

**Table A-3. Default Parameters for  $\beta$ -SOAR Near Field Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
TemperatureAmbient	Ambient temperature (note that ambient temperature increases with depth) (deg. Celsius)	Uniform 20, 30	Not used in this version
fCrossSection_BFtoFracture	Fraction to compute the cross section of the transition region from the backfill material to the closest fracture, using the backfill unit cross section as reference. This parameter is only used if a high diffusive resistance in this transition region is assumed (unitless)	Discrete 1, 1	Flexibility parameter
BF_dispersivityFraction	Dispersivity fraction of a backfill unit after cracking (unitless)	Uniform 0.05, 0.15	Typical range
BFtoFrac_dispersivityFraction	Dispersivity fraction of transition region (unitless)	Uniform 0.1, 0.2	Typical range

**Table A-4. Default Parameters for  $\beta$ -SOAR Far Field Model Component**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
Porosity_Granite	Porosity of Granite (unitless)	Uniform 6.80E-04, 1.50E-03	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. Table A-42 indicates log-10 mean porosity for three different granites ranging from -2.84 to -3.17.
Density_Granite	Bulk Density of Granite (kg/m <sup>3</sup> )	Uniform 2000, 2500	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. Page 125 suggests a generic value of 2600 kg/m <sup>3</sup> is appropriate for modeling as natural variability is not significant.
Porosity_Sediments	Porosity of Sediments (unitless)	Uniform 0.07, 0.3	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-2. Porosity of differentiated valley fill mean value of 0.18 with standard deviation of 0.051. Range given approximates mean plus or minus two standard deviations
Density_Sediments	Bulk Density of Sediments (kg/m <sup>3</sup> )	Uniform 1750, 2070	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-2. Bulk density of alluvium mean value is 1910 kg/m <sup>2</sup> with standard deviation of 78. Range given approximates mean plus or minus two standard deviations.
Kd_Cs_Granite_Ox	Kd of Cs in fractured rock, oxidizing conditions (m <sup>3</sup> /kg)	Log-uniform 4.00E-05, 2.00E-01	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. 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_I_Granite_Ox	Kd of I in fractured rock, oxidizing conditions (m <sup>3</sup> /kg)	Discrete 1, 0	Treated as nonsorbing anion.
Kd_Np_Granite_Ox	Kd of Np in fractured rock, oxidizing conditions (m <sup>3</sup> /kg)	Log-uniform 2.00E-04, 2.20E-02	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. 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.

**Table A-4. Default Parameters for  $\beta$ -SOAR Far Field Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
Kd_Pu_Granite_Ox	Kd of Pu in fractured rock, oxidizing conditions (m <sup>3</sup> /kg)	Log-uniform 0.1, 1	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. 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_Tc_Granite_Ox	Kd of Tc in fractured rock, oxidizing conditions	Discrete 1, 0	Treated as nonsorbing anion
Kd_U_Granite_Ox	Kd of U in fractured rock, oxidizing conditions (m <sup>3</sup> /kg)	Log-uniform 5.00E-05, 1.20E-02	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. 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_C_Granite_Ox	Kd of C in fractured rock, oxidizing conditions (m <sup>3</sup> /kg)	Discrete 1, 0	Treated as nonsorbing anion
Kd_Cs_Sed_Ox	Kd of Cs in porous rock, oxidizing conditions (m <sup>3</sup> /kg)	Log-uniform 100, 1000	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-2. Reference provides minimum and maximum for range. Log-uniform gives equal weight to each order of magnitude of uncertainty range.
Kd_I_Sed_Ox	Kd of I in porous rock, oxidizing conditions (m <sup>3</sup> /kg)	Discrete 1, 0	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-1 identifies iodine as nonsorbing.
Kd_Np_Sed_Ox	Kd of Np in porous rock, oxidizing conditions (m <sup>3</sup> /kg)	Log-uniform 1.8, 13	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-2. Reference provides minimum and maximum for range. Log uniform give equal weight to each order of magnitude of uncertainty range
Kd_Pu_Sed_Ox	Kd of Pu in porous rock, oxidizing conditions (m <sup>3</sup> /kg)	Log-uniform 50, 300	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-2. Reference provides minimum and maximum for range. Log uniform give equal weight to each order of magnitude of uncertainty range
Kd_Tc_Sed_Ox	Kd of Tc in porous rock, oxidizing conditions (m <sup>3</sup> /kg)	Discrete 1, 0	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-1 identifies as nonsorbing

**Table A-4. Default Parameters for  $\beta$ -SOAR Far Field Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
Kd_U_Sed_Ox	Kd of U in porous rock, oxidizing conditions ( $\text{m}^3/\text{kg}$ )	Log-uniform 1.7, 8.9	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-2. Reference provides minimum and maximum for range. Log uniform give equal weight to each order of magnitude of uncertainty range.
Kd_C_Sed_Ox	Kd of C in porous rock, oxidizing conditions ( $\text{m}^3/\text{kg}$ )	Discrete 1, 0	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-1 identifies as nonsorbing
Kd-Cs_Granite_Aniox	Kd of Cs in fractured rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-uniform 4.00E-05, 2.00E-01	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. 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_I_Granite_Aniox	Kd of I in fractured rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Discrete 1, 0	Treated as a nonsorbing anion
Kd_Np_Granite_Aniox	Kd of Np in fractured rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-uniform 4.70E-03, 2	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. 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_Pu_Granite_Aniox	Kd of Pu in fractured rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-uniform 0.1, 1	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. 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_Tc_Granite_Aniox	Kd of Tc in fractured rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Discrete 1, 0	Treated as nonsorbing anion
Kd_U_Granite_Aniox	Kd of U in fractured rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-uniform 4.80E-03, 2.80E-01	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. 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_C_Granite_Aniox	Kd of C in fractured rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Discrete 1, 0	Treated as nonsorbing anion
Kd-Cs_Sed_Aniox	Kd of Cs in porous rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-uniform 100, 1000	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. Table 6.3.10-2. Reference provides minimum

**Table A-4. Default Parameters for  $\beta$ -SOAR Far Field Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
			and maximum for range. Log-uniform gives equal weight to each order of magnitude of uncertainty range.
Kd_I_Sed_Aniox	Kd of I in porous rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Uniform 0, 0.1	Sandia National Laboratories. 2009. Deep Borehole Disposal of High-Level Radioactive Waste. SAND2009-4401. Values from Table 5.
Kd_Np_Sed_Aniox	Kd of Np in porous rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-uniform 1.8, 13	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. 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_Pu_Sed_Aniox	Kd of Pu in porous rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-uniform 50, 300	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. 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_Tc_Sed_Aniox	Kd of Tc in porous rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Uniform 0, 1.0	Sandia National Laboratories. 2009. Deep Borehole Disposal of High-Level Radioactive Waste. SAND2009-4401. Values from Table 5.
Kd_U_Sed_Aniox	Kd of U in porous rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Log-uniform 1.7, 8.9	DOE. 2008. MDL-WIS-PA-000005 REV00: Total System Performance Assessment Model/Analysis for the License Application. 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_C_Sed_Aniox	Kd of C in porous rock, reducing conditions ( $\text{m}^3/\text{kg}$ )	Uniform 0, 2.0	Sandia National Laboratories. 2009. Deep Borehole Disposal of High-Level Radioactive Waste. SAND2009-4401. Values from Table 5.
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 0.1mm ( $10^{-4}$ m) with two orders of magnitude uncertainty on either side.
FF_L1_Length	Length of leg 1 (km)	Constant 1.67	Base case model will consider 5km transport distance over three transport legs at 1.67 km for each leg.
FF_L1_Fracture_Separation	Distance between fractures with advective flow (m)	Log-uniform 5, 500	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. Tables 6-42 and 6-3 provide average flowing interval frequencies for several granite borehole logs. Results indicate mean fracture spacings as

**Table A-4. Default Parameters for  $\beta$ -SOAR Far Field Model Component (continued)**

Parameter Name	Description	Distribution Type & Values	Reference/Rationale
			low as 3m to as high as 600m, but most average spacings on the order of several tens of meters. Log-uniform distribution from 5 to 500m provides a reasonable approximation of these results with median value of 50m.
FF_L1_Hydraulic_Gradient	Hydraulic gradient of leg 1, used to compute flow velocities and flow rates (unitless)	Constant 1.00E-04	Base case will assume gradient of 1e-4. Uncertainty in flow velocity is represented in other parameters such as hydraulic conductivity and fracture aperture used to calculate velocity.
FF_L1_Hydraulic_K_PM	Hydraulic conductivity of leg 1 (m/yr)	Log-uniform 5, 500	SNL (Sandia National Laboratories) 2007. Saturated Zone Site-Scale Flow Model. MDL-NBS-HS-000011 REV 03. Table 7-4 indicates Ksat for combined test intervals in Well EWDP-19D were 0.5 ft/d (55 m/yr). Figure 7-4 plots results of other tests in alluvium and indicates uncertainty within an order of magnitude above and below this value. Loguniform distribution selected to give median of 50m/yr and equal weight to each order of magnitude.
FF_L1_FluidSaturation	Saturation of leg 1 (unitless)	Constant 1	Base case will assume fully saturated conditions.
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 0.1mm ( $10^{-4}$ m) with two orders of magnitude uncertainty on either side.
FF_L2_Length	Length of leg 2 (km)	Constant 1.67	Base case model will consider 5km transport distance over three transport legs at 1.67 km for each leg.
FF_L2_Fracture_Separation	Distance between major fractures with advective flow (m)	Log-uniform 5, 500	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. Tables 6-42 and 6-3 provide average flowing interval frequencies for several granite borehole logs. Results indicate mean fracture spacings as low as 3m to as high as 600m, but most average spacings on the order of several tens of meters. Log-uniform distribution from 5 to 500m provides a reasonable approximation of these results with median value of 50m.



**Table A-4. Default Parameters for  $\beta$ -SOAR Far Field Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
FF_L2_Hydraulic_Gradient	Hydraulic gradient of leg 2, used to compute flow velocities and flow rates (unitless)	Constant 1.00E-04	Base case will assume gradient of 1e-4. Uncertainty in flow velocity is represented in other parameters such as hydraulic conductivity and fracture aperture used to calculate velocity.
FF_L2_Hydraulic_K_PM	Hydraulic conductivity of leg 2 (m/yr)	Log-uniform 5, 500	SNL (Sandia National Laboratories) 2007. Saturated Zone Site-Scale Flow Model. MDL-NBS-HS-000011 REV 03. Table 7-4 indicates Ksat for combined test intervals in Well EWDP-19D were 0.5 ft/d (55 m/yr). 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 50m/yr and equal weight to each order of magnitude.
FF_L2_FluidSaturation	Saturation of leg 2 (unitless)	Constant 1	Base case will assume fully saturated conditions
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 0.1mm (1e-4 m) with two orders of magnitude uncertainty on either side.
FF_L3_Length	Length of leg 3 (km)	Constant 1.67	Base case model will consider 5km transport distance over three transport legs at 1.67 km for each leg.
FF_L3_Fracture_Separation	Distance between major fractures with advective flow (m)	Log-uniform 5, 500	SKB. 2006. Data report for the safety assessment SR-Can. Technical Report TR-06-25. Tables 6-42 and 6-3 provide average flowing interval frequencies for several granite borehole logs. Results indicate mean fracture spacings as low as 3m to as high as 600m, but most average spacings on the order of several tens of meters. Log-uniform distribution from 5 to 500m provides a reasonable approximation of these results with median value of 50m.
FF_L3_Hydraulic_Gradient	Hydraulic gradient of leg 3, used to compute flow velocities and flow rates (unitless)	Constant 1.00E-04	Base case will assume gradient of 1e-4. Uncertainty in flow velocity is represented in other parameters such as hydraulic conductivity and fracture aperture used to calculate velocity.
FF_L3_Hydraulic_K_PM	Hydraulic conductivity of leg 3 (m/yr)	Log-uniform 5, 500	SNL (Sandia National Laboratories) 2007. Saturated Zone Site-Scale Flow Model. MDL-NBS-HS-000011 REV 03. Table 7-4 indicates Ksat for combined test intervals in Well EWDP-19D were 0.5 ft/d (55 m/yr). Figure 7-4 plots results

**Table A-4. Default Parameters for  $\beta$ -SOAR Far Field Model Component (continued)**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
			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 50m/yr and equal weight to each order of magnitude.
FF_L3_FluidSaturation	Saturation of leg 3 (unitless)	Constant 1	Base case will assume fully saturated conditions
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.
FF_DispersivityFraction	Dispersivity expressed as a fraction of the length of the FF transport pathway (unitless)	Discrete 1, 0.1	Base case will assume dispersion length is 10 percent of path length.

**Table A-5. Default Parameters for  $\beta$ -SOAR Biosphere Model Component**

<b>Parameter Name</b>	<b>Description</b>	<b>Distribution Type &amp; Values</b>	<b>Reference/Rationale</b>
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	Table 11 of U.S. Department of Agriculture, National Agricultural Statistics Service, February 2010 report entitled "2008 Farm and Ranch Irrigation Survey, Volume 3, Special Studies, Part 1, 2007 Census of Agriculture." Available at <a href="http://www.agcensus.usda.gov/Publications/2007/Online_Highlights/Farm_and_Ranch_Irrigation_Survey/fris08.pdf">http://www.agcensus.usda.gov/Publications/2007/Online_Highlights/Farm_and_Ranch_Irrigation_Survey/fris08.pdf</a> and accessed on April 30, 2010.
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, 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]	Table A.1 of International Commission on Radiological Protection. Publication 72. "Age-dependent Doses to Members of the Public from Intake of Radionuclides: Part 5, Compilation of Ingestion and Inhalation Dose Coefficients." Elsevier Science, Inc.: Tarrytown, New York. 1996.
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)	Discrete 1, 1	None. Initial value of unity does not change concentration calculation.
Water_Consumption_Rate	Population-averaged consumption rate of well water for adults in the United States (L/yr)	Beta 380, 262, 24, 1023	Table A1, Appendix E, Page E-4 of U.S. Environmental Protection Agency. "Estimated Per Capita Water Ingestion and Body Weight in the United States—An Update." EPA-822-R-00-001. Washington, DC: U.S. Environmental Protection Agency. October 2004.

**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*: A Federally funded research and development center in San Antonio, Texas, sponsored by the U.S. Nuclear Regulatory Commission, to provide the U.S. Nuclear Regulatory Commission 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  $10^{-6}$  meters that are suspended in a solvent. Colloids that are transported in ground water 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*: (1) The spreading or dissemination of a substance caused by concentration gradients. (2) 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 ground water move through the subsurface by means of diffusion because of a concentration gradient.

*dispersion*: (1) The tendency of a solute (substance dissolved in ground water) to spread out from the path it is expected to follow if only the bulk motion of the flowing fluid were to move it. (2) 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: (1) direct release of radioactivity to the surface, or (2) alteration of the nominal behavior of the system.

*dissolution*: (1) Change from a solid to a liquid state. (2) 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*: (1) Occurrences that have a specific starting time and, usually, a duration shorter than the time being simulated in a model. (2) 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 ground-water 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 ground-water 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; and 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 non-useable 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*: 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 the U.S. Nuclear Regulatory Commission 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 electron. The oxidation state is lower in anoxic (reducing) environment 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, a degree of belief.

*probability distribution*: The set of outcomes (values) and their corresponding probabilities for a random variable.

*processes*: PA 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 β-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.

*transport*: A process that allows substances such as contaminants or radionuclides to be carried in a fluid through (1) the physical mechanisms of convection, diffusion, and dispersion; and (2) 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.

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*variable*: A nonunique property or attribute.

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

## **APPENDIX C**

### **Potential Future Development**

NRC staff has identified the following technical areas that may require additional study to support NRC licensing and oversight of potential alternatives for geologic disposal of spent nuclear fuel and high-level waste. These areas complement existing staff knowledge and expertise gained from previous repository experience. Staff will begin to address those issues with broad applicability over multiple potential disposal alternatives consistent with the principles developed in the proposed adaptive framework. Some work in each of these areas, beginning with literature review and understanding of international experience, will start in Fiscal Year 2011.

<b>Table C–1. Potential Future Analyses and Model Support Activities</b>	
Waste Form, Radionuclide Release, and Transport in Different Geologic Environments	Characteristics and performance of alternate waste forms
	Radionuclide release mechanisms from alternate waste forms
	Organic complexation during release and transport
	Radionuclide sorption during release and transport
	Environmental controls on transport processes
	Role of colloids in radionuclide transport
Operational Safety for Alternative Disposal Options	Handling of alternate waste forms during site operations
Geologic Conditions and Site Characteristics of Alternative Disposal Options	Regional geologic conditions and processes
	Regional impacts of future climates
	Disruptive geologic events and natural hazards
	Potential performance of salt as a host rock
Engineered Barrier System Performance in Different Geologic Environments	Waste container materials, characteristics, and degradation
	Performance of buffer and backfill materials
	Performance of cement-based materials
	Microbial effects on materials
	Thermohydrology and near-field coupled processes
Performance Assessment for Alternative Disposal Options	Quantitative evaluation of model uncertainties
	Systematic criteria for assessing features, events, and processes
Assessment of Potential Long-term Impacts for NEPA Assessments	Potential environmental impacts over time periods of expected geologic repository performance