Repository Integration Program

RIP Performance Assessment and Strategy Evaluation Model Theory Manual and User's Guide

RIP is a complex software tool. Proper application of RIP requires an understanding of the underlying principles and assumptions. The importance of reading the associated documentation prior to using the software can not be overemphasized. Before attempting to use the software, it is recommended that the user first read the Theory and Capabilities Manual. This is a large, detailed document and will not necessarily be completely digested in one reading. However, reading through the document once will provide the user with a basic understanding of RIP's capabilities and limitations. Having done so, the user should read this User's Guide. It would be most effective to follow along with RIP loaded on a computer in front of the reader as each part of the software is explained. Although learning to use RIP in the manner outlined above requires a substantial amount of time and effort up-front, this will be more than compensated for in the long-term, and will help ensure appropriate application of the software and meaningful interpretation of results.

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INTRODUCTORY INFORMATION

CONTENTS: This document contains two separate reports: the RIP Theory and Capabilities Manual, and the RIP User's Guide. The former describes the theory and algorithms incorporated into RIP; the latter describes how to actually use the software.

VERSION: RIP is intended to be a code that continually evolves with time, responding to changes in our understanding of the processes controlling the behavior of radioactive waste repositories, and the needs of program users. This document describes Version 4.04 of the RIP software.

SOFTWARE OWNERSHIP: RIP has been developed by Golder Associates Inc. (Golder) over several years. The costs of development have been borne by the US Department of Energy, by other Golder clients internationally, and by Golder itself. Golder takes the position that it has proprietary rights to the software. However, Golder grants the United States Government and others acting on its behalf a royalty-free, nonexclusive, irrevocable world-wide license *for US Governmental purposes* to publish, distribute, translate, duplicate, exhibit and use Version 4.04 of the executable code and the associated documentation.

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ACKNOWLEDGMENTS

RIP was developed by Golder Associates. The software was designed by Ian Miller, Rick Kossik, and Mark Cunnane. Bill Fuget, Ian Miller and Wei Li wrote the computer code for the user interface (the RIP front end). Warren Jones, Bill Fuget and Wei Li wrote the computer code for the computational algorithms of the back end. The documentation was written by Rick Kossik, Mark Cunnane, Ian Miller, Joe Hachey, Alan Keizur and Dawn Shuttle.

RIP incorporates concepts from a number of individuals who generously gave of their time to attend a series of workshops held by Golder Associates in 1991 and 1992. The workshops were attended by representatives from Lawrence Livermore National Laboratory (which hosted one of the workshops), Sandia National Laboratories, Los Alamos National Laboratory, the U.S. Geological Survey (USGS), Lawrence Berkeley Laboratory, RE/SPEC, Battelle Pacific Northwest Laboratory, Science Applications International Company (SAIC), Roy F. Weston Inc., Electric Power Research Institute (EPRI), Yucca Mountain Site Characterization Project Office (YMP), Mifflin and Associates, Geomatrix Consultants, Intera Sciences, University of Minnesota, and the Georgia Institute of Technology. We would like to thank these organizations for their input, without which this model could not have been developed.

Although input from the organizations listed above was utilized in the design of RIP, Golder Associates formulated the computational structure of the model independently and is solely responsible for the contents of this document.

RELEASE NOTES FOR RIP VERSION 4.04

RIP is intended to be a code which continually evolves with time, responding to changes in our understanding of the processes controlling the behavior of waste disposal systems, and the needs of program users.

Subsequent revisions to Version 4.04 of RIP will be named as follows:

- Modifying the version number by 0.01 (e.g., from 4.04 to 4.05) indicates correction of a minor bug (or bugs);
- Modifying the version number by 0.1 (e.g. from 4.04 to 4.10) indicates correction of a more important bug or addition of another feature.

Golder will send new releases of RIP to registered users along with a Release Notes page that explains the change(s). The Release Notes page will include the following:

- the date
- the new version number (e.g., 4.04)
- the version number which is being replaced (e.g., 4.04)
- an explanation of the changes or modifications that were made

The user should insert the new Release Notes immediately following this page.

In addition, if the revisions to the RIP software require changes to the RIP manuals, Golder will send replacement pages for the manuals (as appropriate) along with an Interim Change Notification (ICN) form to registered users. The ICN will document which pages were replaced. The user should file the ICN behind the Release notes. The ICNs and replacement pages will remove the necessity to re-issue the entire RIP manual with each new release of RIP. However, the RIP manuals will be re-issued if the changes are sufficiently far-reaching to warrant a re-issue or if the cumulative number of ICNs warrant a re-issue.

The authors request that users who have identified a bug in the code please send a *RIP Software Problem Report* (included in Appendix D of the User's Guide), along with a disk containing the RIP input file, to:

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**RIP REPOSITORY PERFORMANCE ASSESSMENT
AND STRATEGY EVALUATION MODEL:**

THEORY AND CAPABILITIES

Version 4.04

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ABSTRACT

This report describes the theory and capabilities of RIP (Repository Integration Program). RIP is a powerful and flexible computational tool for carrying out probabilistic integrated total system performance assessments for geologic repositories.

The primary purpose of RIP is to provide a management tool for guiding system design and site characterization. In addition, the performance assessment model (and the process of eliciting model input) can act as a mechanism for integrating the large amount of available information into a meaningful whole (in a sense, allowing one to keep the "big picture" and the ultimate aims of the project clearly in focus). Such an integration is useful both for project managers and project scientists.

RIP is based on a "top down" approach to performance assessment that concentrates on the integration of the entire system, and utilizes relatively high-level descriptive models and parameters. The key point in the application of such a "top down" approach is that the simplified models and associated high-level parameters must incorporate an accurate representation of their uncertainty. RIP is designed in a very flexible manner such that details can be readily added to various components of the model without modifying the computer code. Uncertainty is also handled in a very flexible manner, and both parameter and model (process) uncertainty can be explicitly considered. Uncertainty is propagated through the integrated PA model using an enhanced Monte Carlo method.

RIP must rely heavily on subjective assessment (expert opinion) for much of its input. The process of eliciting the high-level input parameters required for RIP is critical to its successful application. As a result, in order for any project to successfully apply a tool such as RIP, an enormous amount of communication and cooperation must exist between the data collectors, the process modelers, and the performance assessment modelers.

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EXECUTIVE SUMMARY

Introduction

This report provides a detailed description of the theory and capabilities of RIP (Repository Integration Program), an integrated performance assessment and strategy evaluation model for radioactive waste repositories. RIP was originally developed for application to the potential high-level radioactive waste repository at Yucca Mountain, Nevada. *Its use, however, is not necessarily limited to this particular site.* This is because, for the most part, RIP is designed in a very flexible manner. In simple terms, *RIP is a simulation tool designed to probabilistically model the release of radionuclides from disposal sites and the subsequent transport of those radionuclides through the environment.* Because the physical processes that are built into the RIP algorithms are relatively fundamental and not site specific, the software could be applied to a variety of sites.

The major portion of the software is the total system performance assessment model, which consists primarily of a series of inter-connected, coupled component models with input/output relationships for radionuclide transfer. The performance model itself is embedded within a probabilistic decision analysis model that allows the user to evaluate alternative site characterization strategies.

This report defines the overall methodology on which the program is based and describes the actual algorithms embodied within the software. It does *not* specifically describe the application of the software to any specific site.

Overview of Methodology

The Role of Performance Assessment

Traditionally, performance assessment has been considered as an essential method to be implemented at the later stages in a repository siting program, after the site has been characterized. However, performance assessment can also be used as a tool to aid in the development and implementation of the entire siting and design procedure. In fact, Golder Associates (Golder) and others have long maintained that the only effective way to make valid site characterization decisions (what should be studied, when, and in what detail) and to improve conceptual designs is by using preliminary integrated performance assessments. This view has been reiterated by both the National Research Council (1990) and the Nuclear Waste Technical Review Board (1990).

This view of an ongoing performance assessment-driven characterization and design process is based on the premise that by evaluating system performance using *currently available knowledge* and the *anticipated level of knowledge that can be obtained following completion of a characterization or design activity*, it will be possible to identify which activities will be most critical to rapid and accurate determination of site suitability. That is, integrated performance assessment is intended to be used in an ongoing review process to continually reevaluate which data needs are most critical, and to reallocate program resources appropriately. Figure ES-1 illustrates the intended process graphically.

FIGURE **ES-1**
METHODOLOGY OVERVIEW
ARGONNE/MODEL DEVELOPMENT

The Performance Assessment Model

At the heart of the Golder methodology is the integrated total system performance assessment model. It is Golder's belief that a practical performance assessment model based completely on low-level physically-based parameters is not currently feasible. That is, the uncertainty in quantifying the basic physical processes controlling waste release, groundwater flow, and radionuclide transport at any real site is such that a practical performance assessment model must rely on relatively high-level "lumped" descriptive parameters (e.g., radionuclide travel times, container failure rates), which in turn are based on lower-level "process" models and on subjective assessments from qualified experts.

Moreover, it is Golder's view that due to computational constraints and the inherent complexity of such systems, it is unlikely that this situation will change in the foreseeable future. Although better simulation tools, more powerful computers, and additional field data will undoubtedly shed considerable light on the controlling processes, integrated total system performance models will continue to rely primarily on high-level parameters. Additional detailed process modeling and field studies will simply act to increase the accuracy and decrease the uncertainty in the experts' subjective assessments of these parameters.

As a result, the total system performance assessment model incorporated into RIP is *not* a detailed deterministic model based completely on low-level physically-based parameters (e.g., it does not explicitly simulate radionuclide transport by solving a three-dimensional advection-diffusion equation). Rather, it is a *descriptive probabilistic model* based on a "top down" approach to performance assessment that *describes* rather than *explains* the system behavior and is intended to directly represent the uncertainties in processes and events and their controlling parameters. This is not to say that detailed models of the controlling processes are ignored. Quite to the contrary, detailed process models form the foundation for a systems model such as RIP and are required to generate the appropriate input parameters (e.g., in the form of response surfaces or analytical expressions).

The structure and concepts of the integrated total system performance assessment model will be discussed in greater detail below.

Evaluating Alternative Strategies

As discussed above, the integrated performance assessment model is intended to be used as a tool to make valid design and site characterization decisions and to identify which activities will be most critical to rapidly and accurately determining site suitability.

After first developing a conceptualization of the behavior of a repository system and creating an appropriate data set for the integrated performance assessment model, it is possible to apply the tool to guide site characterization. In order to accomplish this, however, it is first necessary to identify which system parameters and processes are specifically addressed by the various characterization or design *activities*. A characterization or design activity is a specific scientific study or group of studies proposed for the site (e.g., surface-based testing, laboratory testing of container corrosion rates).

In order to most effectively use performance assessment to guide site characterization and design, however, it is necessary not only to identify *which* parameters would be affected by a particular activity, but to quantify *how* those parameters would be affected. In effect, this entails quantifying how a proposed activity is likely to affect the probability distribution describing the uncertainty in a given system parameter (i.e., how much will we learn?). This requires evaluations by experts of the nature of the uncertainty in a parameter, and the extent to which it is likely to be resolved by a particular activity.

An *activities database* must be developed, which includes the name of each proposed activity, a brief description, identification of the system parameters the activity will affect, a quantitative estimate of how those parameters will be affected, probabilistic estimates of cost and duration of the activity, and precedence requirements for other activities.

Having developed an activities database, the simplest way to use RIP to evaluate characterization and design activities is to evaluate the results of a performance assessment such that the sensitivities of various system performance measures (e.g., cumulative radionuclide release to the accessible environment, peak individual dose) to individual model parameters are identified. In simple terms, activities that provide information on model parameters to which system performance is sensitive should be given the highest priority.

Although such an approach is useful in providing a preliminary screening and evaluation of site activities, it is limited because while it qualitatively considers which parameters are affected by a particular activity, it does not quantitatively incorporate the extent to which parameter uncertainty might be reduced by a particular activity, nor the cost or duration of the activity. This information is required in order to actually *prioritize* activities into an efficient and effective strategy. For example, suppose two proposed activities are both concerned with studying a particular parameter that has been shown to have a strong influence on system performance. While we can state that these activities both merit further consideration, we can not determine whether both activities are necessary, or which would be most effective, without quantifying the extent to which each activity will reduce the uncertainty in system performance, and incorporating cost and duration considerations.

Moreover, because of the complexity of the system and the large number of inter-connected activities, actual prioritization of activities can not be based simply on an evaluation of individual activities with respect to cost, duration, and reduction in performance uncertainty. Rather, the entire site characterization plan must be considered as a whole. The proposed methodology accomplishes this prioritization by defining and evaluating *alternative characterization strategies* (a characterization strategy consisting of a specific set or sequence of characterization activities). The strategy portion of RIP provides the second cornerstone of the Golder approach by quantitatively integrating the performance assessment model with the characterization and design activities. The strategy model is essentially a decision analysis shell around the performance assessment model that allows the user to evaluate the alternative site characterization strategies.

The performance assessment model and the strategy evaluation model are discussed in more detail below.

Performance Assessment Model Overview

Basic Concepts

The integrated total system performance model consists of four coupled components that address:

- waste package behavior and radionuclide release;
- fluid flow and radionuclide transport through the geosphere;
- disruptive events (such as volcanism and human intrusion) that can affect system parameters; and
- radionuclide fate and effect (dose/risk) in the biosphere.

Figure ES-2 is a schematic of the performance assessment model structure.

As pointed out previously, RIP is a *descriptive* model that relies heavily on subjective assessments of relatively high-level descriptive parameters. It is also a *probabilistic* model intended to represent the uncertainties in processes and events. That is, uncertainty in both the model parameters and the component models themselves can be explicitly represented by RIP. Due to the inherent uncertainties resulting from our lack of knowledge, many model parameters will be represented by probability density functions (pdfs). The integrated performance assessment model uses a *simulation approach*, utilizing the Monte Carlo method to sample the probability distributions for the uncertain parameters (describing both processes and events) and simulate a large number of system realizations in order to determine probability distributions of site performance (e.g., cumulative release). That is, RIP creates a time history of disruptive events and other system parameters for each system realization, simulates the behavior of the system under those conditions, and then combines the results of all the realizations in an appropriate manner to determine probability distributions of site performance. RIP utilizes both *importance sampling* and *stratified (Latin-Hypercube) sampling* to increase the efficiency of the Monte Carlo sampling process.

In general terms, the output for the performance assessment model consists of performance measures for the repository system. A variety of performance measures can be considered (e.g., cumulative radionuclide release to the accessible environment, maximum annual release from the waste packages, peak individual dose). These performance measures are probabilistic in nature. That is, output is not a single value, but a distribution that specifies the probability of exceedance for any particular value of a performance measure.

FIGURE **ES-2**
RIP PERFORMANCE ASSESSMENT MODEL COMPONENTS
 ARGONNE/MODEL DEVELOPMENT

Flexibility of the Software

A fundamental feature of the RIP methodology, which is critical to understand in order to appreciate the power and flexibility of the software, is the concept that a given model parameter can be specified by the user as a *constant*, a *stochastic* (i.e., represented by a probability distribution), or as a *function of time or of other parameters* (which themselves can be constants, stochastics, or functions).

Representing system parameters as stochastics allows the RIP user to directly specify the degree of uncertainty in a particular parameter. The RIP user interface (which consists of a series of interactive menus and pop-up input windows) allows the user to choose from a wide variety of probability distributions. For each Monte Carlo realization of the repository system, all of the stochastic parameters are sampled from their specified distributions. The probability distributions used for stochastic parameters can themselves be stochastic, or functions of other parameters.

The ability to represent system parameters as functions of other parameters imparts to the user the ability to readily add detail to any given system parameter or process represented by RIP. The user can even create and specify processes and parameters that are not explicitly incorporated in RIP. In a sense, the RIP program is similar to a spreadsheet: while it contains a large amount of built-in logic and calculational capabilities, the problem that is solved is entirely defined by the user. That is, RIP has been developed such that it consists of a basic computational framework representing the controlling processes, but is intentionally flexible such that the user can represent the processes with as much detail as desired.

The user interface of the software is designed such that for function-type parameters the user types in the desired function. In addition to standard mathematical operators (e.g., SIN, COS, MAX, ERF, LOG), the user can define functions using relational operators (e.g., >, <, =) and IF, THEN logic. Such flexibility allows the user to easily modify and add detail to the conceptual and computational model *without having to make changes to the software* (i.e., without modifying and compiling the source code). This allows the conceptual model to be continuously and easily modified as more information becomes available. For more complex functions, the software is structured such that the user can develop separate *coded functions* (i.e., separate coded program modules, written in the C programming language) which can then be directly coupled with the main RIP algorithms.

Components of the Performance Assessment Model

The major features of the four component models that comprise the performance assessment model are summarized briefly here.

The *waste package behavior and radionuclide release component* requires as inputs descriptions of the radionuclide inventories in the waste packages, a description of near field environmental conditions (which may be defined as temporally and spatially variable), and subjective assessments of high-level parameters describing container failure, matrix alteration/dissolution, and radionuclide mass transfer. The waste package component model can simulate two layers of containment (e.g., outer package and zircalloy cladding). Waste package failure rates, along

with matrix alteration/dissolution rates, are used to compute the rate at which radionuclides are *exposed*. Once exposed, RIP computes the rate of *mass transfer* out of and away from the waste package. Parameters describing waste package failure and radionuclide exposure and mass transfer can be described as a function of near-field environmental conditions.

The output from this component (for each system realization) consists of time histories of release for each radionuclide from the waste packages, and acts as the input for the transport pathways component.

The task of the *radionuclide transport pathways component* is to probabilistically simulate radionuclide transport through the near and the far field. Workshops held by Golder indicated that existing continuum-based models, while representing portions of a system well, *often fail to capture the essence of complex hydrologic systems*. While this may change in the future, the current model must be capable of representing what is known about a site *at the present time*. Thus, the RIP model uses a phenomenological approach that attempts to *describe* rather than *explain* the system.

The resulting transport algorithm is based on a network of user defined *pathways*. The geosphere and biocell pathways reflect the major features of the hydrologic system and the biosphere, and are conduits through which transport occurs. The pathways may be used for both flow balance and radionuclide transport purposes, and may account for either gas or liquid phase transport. The purpose of a pathway is to represent large scale heterogeneity of the hydrologic system, such as geologic structures and formation scale stratigraphy. In highly complex systems (such as Yucca Mountain), many pathways may be required.

Geosphere pathways may be subdivided into *flow modes*, which address heterogeneity at the local scale (e.g., flow in rock matrix, flow in fractures). The flow modes are primarily distinguished from one another based on flow velocity in the mode, although retardation parameters may also differ between flow modes.

The actual transport of radionuclides along a geosphere pathway is based on a *breakthrough curve*, which is developed as a cumulative probability distribution for radionuclide travel times along the pathway. The breakthrough curve combines the effects of all flow modes and retardation on the radionuclide travel time, and determines the expected proportion of mass that has traversed the pathway by any specified time. The breakthrough curve is computed based on a Markov process algorithm for exchange between different flow modes.

The third performance assessment component model represents *disruptive events*. Disruptive events are defined as discrete occurrences that have some quantifiable effect on the processes described by the other two component models. Examples of disruptive events include volcanism, faulting, and human intrusion. The user first identifies all *significant events* (i.e., events that are both credible and consequential). Having done so, each event is assigned a rate of occurrence and, if desired, one or more *descriptor parameters*, which define the characteristics and magnitude of the event (e.g., length of a volcanic dike). Descriptor parameters may be described stochastically. Event occurrences are simulated as Poisson processes.

The user defines probability distributions for the event *consequences* (which may be functions of event descriptors). A consequence may take the form of a number of *discrete responses* (e.g., disrupting a number of waste packages, moving radionuclides from some waste packages directly to the accessible environment). It is also possible for an event to directly modify parameters defined in the other two component models, and this capability can be used to specify *long-term consequences* (e.g., raising the water table or opening a new pathway).

The fourth performance assessment component model describes the fate and effect of radionuclides in the biosphere. The *biosphere dose/risk model* allows the user to define *dose receptors* in the system. Receptors receive doses from specified geosphere (e.g., a water supply aquifer) or biosphere (e.g., a pond, or flora and fauna) pathways. Concentrations in these pathways are converted to doses (or cancer risks) based on user-defined conversion factors.

Strategy Evaluation Model Overview

The performance assessment model is embedded within a decision analysis model that allows the user to evaluate alternative site characterization strategies, where a strategy is defined as a group of activities. Figure ES-3 provides a schematic of the RIP strategy evaluation model.

For any user-specified characterization strategy, RIP provides three outputs by which alternative strategies can be ranked and compared:

- a probabilistic estimate of cost;
- a probabilistic estimate of duration; and
- a probabilistic evaluation of the predicted site performance resulting from implementation of the strategy (i.e., "what will our performance predictions be after we carry out this strategy?").

Computation of the first two outputs is straightforward, and consists of integrating within a Monte Carlo framework the cost and duration estimates for the individual activities, taking into account any precedence requirements. The third output relies on subjective assessments by experts of the extent to which model parameter uncertainty will be reduced by a particular activity. Given these assessments, along with the current state of knowledge, RIP uses a Bayesian computational algorithm to simulate how probability distributions representing parameter uncertainty will change as a result of a particular characterization strategy, and develops a probabilistic evaluation of the anticipated repository performance that will be predicted after carrying out the strategy. Based on these outputs, it is possible to evaluate that effectiveness of alternative site characterization strategies.

FIGURE **ES-3**
OVERVIEW OF RIP
STRATEGY EVALUATION
 ARGONNE/MODEL DEVELOPMENT

Model Application

As discussed above, the primary objective of RIP is to provide a management tool for guiding design and site characterization. A related and equally important use for the model has become apparent to Golder in the process of eliciting information regarding models and input data from scientists and engineers in various international programs. Namely, the performance assessment model (and the process of eliciting model input) can act as a mechanism for integrating the large amount of available information generated by different groups into a meaningful whole (in a sense, allowing one to keep the "big picture" and the ultimate aims of the project clearly in focus). Such an integration is not only useful for project managers (and is ultimately required in order to carry out a meaningful assessment of site suitability), but also to individual project scientists to help them formulate and present the results of their research in a manner such that it can be *readily applied* to the ultimate goal of the any disposal project, *predicting the performance and determining the suitability of the site*.

RIP must rely heavily on subjective assessment (expert opinion) for much of its input. The process of eliciting the high-level input parameters required for RIP is critical to its successful application. As a result, in order for any project to successfully apply a tool such as RIP, an enormous amount of communication and cooperation must exist between the data collectors, the process modelers, and the performance assessment modelers. This is because such a tool must constantly evolve and is only valid for decision making when it actually incorporates the *current state of knowledge*. This is only possible if project scientists and engineers *think in terms of performance assessment*, at least to the extent that their results can be readily incorporated into a total system model. In effect, they must be familiar with that portion of the total system performance assessment model that represents the particular process or parameter that they are studying, such that they can recommend modifications in the data (or the model itself if necessary) as more information becomes available.

Without this type of integration between the performance assessment modelers and the project scientists, a tool such as RIP can not be validly applied.

1. INTRODUCTION

This report provides a detailed description of the theory and capabilities of RIP (Repository Integration Program), an integrated performance assessment and strategy evaluation model for radioactive waste repositories. RIP was originally developed for application to the potential high-level radioactive waste repository at Yucca Mountain, Nevada. *Its use, however, is not necessarily limited to this particular site.* This is because, for the most part, RIP is designed in a very flexible manner. In simple terms, *RIP is a simulation tool designed to probabilistically model the release of radionuclides from disposal sites and the subsequent transport of those radionuclides through the environment.* Because the physical processes that are built into the RIP algorithms are relatively fundamental and not site specific, the software could be applied to a variety of sites.

The major portion of the software is the total system performance assessment model, which consists primarily of a series of inter-connected, coupled component models with input/output relationships for radionuclide transfer. The performance model itself is embedded within a probabilistic decision analysis model that allows the user to evaluate alternative site characterization strategies.

This report focuses only on the *theory and capabilities* of the RIP computer program. It is not a user's manual, nor does it discuss the application of the model to any specific site. A user's manual has been prepared as a separate companion document.

In the following section, a brief overview of the RIP methodology is presented. Section 1.2 discusses the organization of the remainder of the report.

1.1 Overview of RIP Methodology

1.1.1 Problem Definition

Programs for selecting and evaluating the suitability of geologic sites for disposal of high level radioactive waste all include three general components: site selection and characterization, system design, and performance (safety) assessment. *Site selection or characterization* activities are primarily concerned with determining the ability of the natural barrier (the geosphere) to provide containment and to control migration of radionuclides from the repository. *System design* is concerned with the ability of the engineered barrier system (EBS), which consists of the waste package itself and the associated man-made systems, to provide containment and control migration. Obviously, site characterization and system design are not independent of each other. That is, the performance of the engineered barrier system is dependent on characteristics of the geologic system, and the characteristics of the geologic system can be altered and affected by the engineered barrier system. As a result, site characterization includes activities that are intended to provide input for the system design.

In simple terms, *performance assessment* involves the evaluation of the anticipated performance of a proposed repository with respect to radionuclide release to the environment (which then may be translated to a dose or risk). It ultimately depends upon both the available data (obtained

during laboratory studies or site characterization) and the proposed engineered barrier system design.

The task of performance assessment is complicated by the large uncertainties involved. Due to the long time scales of interest and the complexity of most geologic systems, a large degree of uncertainty exists with respect to the parameters and processes controlling such a system. As a result of these uncertainties, Golder Associates believes that deterministic analysis alone is typically inappropriate and a probabilistic approach to performance assessment must be used.

1.1.2 The Role of Performance Assessment

Traditionally, performance assessment has been considered as an essential analysis to be implemented at the later stages in a repository program in order to demonstrate that the candidate site is in compliance with the licensing criteria. Performance assessment, however, can also be used as a tool to aid in the development and implementation of the entire siting and design procedure. In fact, Golder Associates and others have long maintained that the only effective way to make valid site selection, characterization and design decisions (what should be studied, when, and in what detail) is by using preliminary iterative total system performance assessments (e.g., Golder Associates, 1977; NRC, 1983; Golder Associates, 1986). This view has recently been reiterated in the United States by both the National Research Council (1990) and the Nuclear Waste Technical Review Board (1990), and internationally by the NEA (1991).

This view of an ongoing iterative performance assessment-driven design and characterization process is based on the premise that by evaluating system performance using *currently available knowledge and the anticipated level of knowledge that can be obtained following completion of a site selection, characterization, or design activity*, it will be possible to identify which activities will be most critical to rapid and accurate determination of site and design suitability. Figure 1-1 illustrates the intended process graphically.

The RIP methodology has a two-fold purpose:

- to provide a systematic framework for organizing and quantifying the current knowledge (and uncertainty) regarding the performance of the entire repository system; and
- to act as a management tool to aid decision making (e.g., regarding site selection, characterization and design issues) and to help assure continuing program refinement.

The first item listed above has become very apparent to Golder Associates in the process of eliciting information regarding models and input data from scientists and engineers involved in several international repository programs. Namely, the performance assessment model (and the process of eliciting model input) can act as a mechanism and framework for integrating the available information generated by different groups into a meaningful whole (allowing one to keep the "big picture" and the ultimate aims of the project clearly in focus). Such an integration is not only useful for project managers (and is ultimately required in order to carry out a

FIGURE 1-1
METHODOLOGY OVERVIEW
ARGONNE/MODEL DEVELOPMENT

meaningful assessment of site suitability), but can also help individual project scientists and engineers formulate and present the results of their research in a manner such that it can be *readily applied* to the ultimate goal of the project, *predicting the performance and determining the suitability of a selected site*.

The second item simply states that a tool such as RIP can be used in an ongoing review process to continually re-evaluate which data needs are most critical, and to reallocate program resources appropriately.

1.1.3 Performance Assessment Modeling Approach

In general terms, performance assessments can be broadly divided into two categories: those based on a "top down" approach, and those based on a "bottom up" approach. RIP is based on a "top down" approach.

"Bottom up" approaches to performance assessment attempt from the outset to model the various controlling processes in detail, and typically make use of complex *process-level models* for the various system components. The emphasis is on understanding and explaining the processes in great detail in order to eventually describe the behavior of the entire system. Due to the complexity of real systems, however, properly implementing and integrating the various process-level component models and examining total system behavior *while incorporating uncertainty* can be quite difficult. Moreover, under a "bottom up" approach, a large amount of time and money can be inadvertently spent studying processes and parameters that are of little or no importance to repository performance.

As a result, Golder Associates believes that although detailed process-level modeling is ultimately required for credible performance assessments, this detailed modeling should be organized and structured at a higher level using a "top down" approach.

Rather than starting at the bottom and attempting to simulate the physical processes in great detail, "top down" approaches to performance assessment start from the top and concentrate on the *integration* (at a much higher level) of all system components. The controlling processes may initially be represented by approximate high-level (i.e., less detailed) models and parameters. In general, these high-level parameters will take the form of subjective assessments (of probability distributions) from qualified experts.

There are two key points in the application of a "top down" performance assessment approach:

- 1) Less detailed component models and associated high-level parameters must incorporate an accurate representation of the *model and parameter uncertainty* resulting from the approximations.
- 2) As opposed to representing all processes with great detail from the outset (whether or not it is justified), details are only added when it is warranted (e.g., if additional data is available and results indicate that performance is sensitive to a process that is currently represented in a simplified manner with a correspondingly large degree of

uncertainty). That is, details are only added to those processes that are identified as being important with respect to system performance.

As mentioned above, in a "top down" approach, each system component may initially be represented at a relatively high level. The total system model can then evolve by adding detail (and reducing uncertainty) for specific components as further information becomes available. Such an approach can help to keep a project focused on total system performance without getting lost in what may prove to be unnecessary details.

It is important to understand that a "top down" model does not have to be "simple". Whereas a "simple" model might completely *ignore* a key process, a well designed "top down" model *approximates* the process while explicitly incorporating (using probability distributions) the resulting uncertainty that is introduced.

Although detailed process-level models may not be directly implemented when using such a "top down" approach, this is not to say that detailed modeling is not required. Quite to the contrary, detailed process-models form the foundation for a "top down" total system model such as RIP and are required in order to generate the appropriate input parameters for the top-level model. These input parameters may be in the form of analytical expressions or response surfaces developed by an expert based on detailed modeling results. That is, in formulating the high-level input, the expert will typically base his or her opinion as to the value and the associated uncertainty of a parameter or model on available detailed process-model (or experimental) results.

Figure 1-2 schematically presents the information flow within a "top down" performance assessment approach. Note that information must flow in both directions. At the base of the system are process-level models and field and laboratory experiments. This information is then assimilated by experts into a form that can be used in a total system model. The downward flow of information from the total system model consists of identification of the processes and parameters to which system performance is sensitive and a request for further information.

It is clear from the previous discussion that the process of obtaining subjective assessments from experts (i.e., eliciting expert opinion) is critical to the successful application of a "top down" performance assessment approach. Appendix A outlines the methods for obtaining defensible subjective probability assessments.

FIGURE 1-2
**TOP-DOWN PERFORMANCE
ASSESSMENT INFORMATION FLOW**
ARGONNE/MODEL DEVELOPMENT

1.1.4 The Computational Tool

Due to the uncertainty in quantifying the basic physical processes controlling waste release, groundwater flow, and radionuclide transport over the large time scales of interest, Golder Associates believes that a practical performance assessment model based completely on low-level physically-based models and parameters (a "bottom up" approach) is extremely difficult and computationally intensive. Although detailed deterministic models can provide insight into the controlling processes, they cannot be used to provide a probabilistic analysis of system performance. That is, a practical total system performance assessment model must incorporate a "top down" approach and rely, to a large degree, on high-level parameters based on expert opinion.

Moreover, it is our view that due to computational constraints and the inherent complexity of such systems, it is unlikely that this situation will change much in the foreseeable future. Although better simulation tools, more powerful computers, and field and laboratory data will undoubtedly shed light on the controlling processes, integrated total system performance models will continue to rely primarily on high-level parameters representing expert opinion. Additional detailed process modeling and experiments will simply act to increase the accuracy and decrease the uncertainty in the experts' subjective assessments.

As a result, the total system performance assessment tool in which the above concepts are embodied (the Repository Integration Program - RIP) is not a detailed deterministic model based completely on low-level, physically-based parameters (e.g., it does not explicitly simulate radionuclide transport by solving a three-dimensional advection-diffusion equation). Rather, it is a *descriptive probabilistic model* that acts as an integrating tool for a "top down" performance assessment approach. It *describes* rather than *explains* system behavior and is intended to directly represent the uncertainties in processes and events and their controlling parameters.

The structure and components of the integrated total system performance assessment model incorporated into RIP are described in detail in subsequent chapters.

1.1.5 Development of an Activities Database

As discussed above, the integrated performance assessment model is intended to be used as a tool to make valid site characterization and design decisions and to identify which activities will be most critical to rapidly and accurately determining site suitability.

After first developing a conceptualization of the behavior of the repository system and creating an appropriate data set for the integrated performance assessment model, it is possible to apply the tool to guide site characterization and design. In order to accomplish this, however, it is first necessary to identify which system parameters and processes are specifically addressed by the various characterization or design *activities*. An activity is defined here as a specific scientific or engineering study or group of studies proposed for the site (e.g., surface-based testing, laboratory testing of container corrosion rates). A characterization *strategy* is a specified set of characterization and design activities.

In order to most effectively use performance assessment to guide site characterization and design, however, it is necessary not only to identify *which* parameters would be affected by a particular activity, but to quantify *how* those parameters would be affected. In effect, this entails quantifying how a proposed activity is likely to affect the probability distribution describing the uncertainty in a given system parameter (i.e., how much will we learn?). This requires evaluations by experts of the nature of the uncertainty in a parameter, and the extent to which it is likely to be resolved by a particular activity.

An *activities database* must be developed, which includes the name of each proposed activity, a brief description, identification of the system parameters the activity will affect, a quantitative estimate of how those parameters will be affected, probabilistic estimates of cost and duration, and precedence requirements for other activities.

1.1.6 Evaluating Characterization/Design Activities and Strategies

Having developed an activities database, the simplest way to use RIP to evaluate characterization and design activities is to post-process the results of a performance assessment such that the sensitivities of various system performance measures (e.g., cumulative radionuclide release to the accessible environment) to individual model parameters are identified. In simple terms, activities that provide information on model parameters to which system performance is sensitive should be given the highest priority.

Although such an approach is useful in providing a preliminary screening and evaluation of site activities, it is limited because while it qualitatively considers which parameters are affected by a particular activity, it does not quantitatively incorporate the extent to which parameter uncertainty might be reduced by a particular activity, nor the cost or duration of the activity. This information is required in order to actually *prioritize* activities into an efficient and effective strategy. For example, suppose two proposed activities are both concerned with studying a particular parameter that has been shown to have a strong influence on system performance. While we can state that these activities both merit further consideration, we can not determine whether both activities are necessary, or which would be most effective, without quantifying the extent to which each activity will reduce the uncertainty in system performance, and incorporating cost and duration considerations.

Moreover, because of the complexity of the system and the large number of inter-connected activities, actual prioritization of activities can not be based simply on an evaluation of individual activities with respect to cost, duration, and reduction in performance uncertainty. Rather, the entire site characterization and design plan must be considered as a whole. The proposed methodology accomplishes this by defining and evaluating *alternative characterization strategies* (a characterization strategy consisting of a specific set or sequence of characterization activities). The strategy portion of RIP provides the second cornerstone of the Golder approach by quantitatively integrating the performance assessment model with the characterization activities. The strategy model is essentially a decision analysis shell around the performance assessment model that allows the user to evaluate the alternative site characterization strategies.

For any user-specified characterization strategy, RIP provides three outputs by which alternative strategies can be ranked and compared:

- a probabilistic estimate of cost;
- a probabilistic estimate of duration; and
- a probabilistic evaluation of the predicted site performance resulting from implementation of the strategy.

Computation of the first two outputs is straightforward, and consists of integrating within a Monte Carlo framework the cost and duration estimates for the individual activities, taking into account any precedence requirements. The third output relies on subjective assessments by experts of the extent to which model parameter uncertainty will be reduced by a particular activity. Given these assessments, along with the current state of knowledge, RIP uses a Bayesian computational algorithm to simulate how probability distributions representing parameter uncertainty will change as a result of a particular characterization strategy, and develops a probabilistic evaluation of the anticipated repository performance (i.e., probabilities of future repository performance results).

It should be noted that the degree to which such a methodology can be used to prioritize site characterization activities is inherently limited by the level of detail included in the performance assessment model. For example, it may be possible to determine, based on model results, that with respect to determining site suitability, further information regarding process A would be more beneficial than further information regarding process B. This would imply that activities that obtain information on process A should be given higher priority than those related to process B, and would be a useful finding. However, in order to further prioritize the various activities that specifically investigate the details of process A, it may be necessary to add additional detail to that particular component of the performance assessment model.

Details of both the performance assessment model and the strategy evaluation model are presented in subsequent chapters.

1.2 Report Organization

Chapter 2 discusses the basic concepts of the RIP performance assessment and strategy evaluation model. This provides a summary description of the various features and components of RIP. Readers interested only in the basic features and concepts of the model may wish to read only Chapter 2. Chapters 3, 4 and 5 discuss the details of the three major components of the RIP performance assessment model: waste package behavior and release, radionuclide transport pathways, and disruptive events. Chapter 6 describes the dose/risk modeling options in RIP. Chapter 7 describes the details of the strategy evaluation model. References are listed in Chapter 8.

The report also includes a number of appendices. These appendices describe additional details pertaining to the RIP model and are referenced in the main text.

2. BASIC CONCEPTS OF THE REPOSITORY INTEGRATION PROGRAM (RIP)

Having introduced in very general terms the overall philosophy and methodology upon which RIP is based, in this chapter a more detailed description of the basic concepts of the RIP software are presented. Section 2.1 first discusses some terminology that is used throughout the report. Section 2.2 then describes the structure and fundamental concepts of the performance assessment model, including an overview of each of the four major model components. The structure and fundamental concepts of the strategy evaluation model are discussed in Section 2.3. Section 2.4 discusses the flexibility of the RIP software, which imparts tremendous power to the model. Finally, Section 2.5 provides a summary of the key features of RIP.

2.1 Terminology

The experienced reader will note that the term "model" is used somewhat loosely in this report. Because modeling and simulation terminology is generally not used uniformly throughout the engineering and scientific community, it is important to clearly define at the outset our set of terminology. In particular, it is important to differentiate between what we refer to as the *computational model*, the *conceptual model*, and the *simulation model*.

As used here, the computational model is the tool that provides the mathematical and computational framework for modeling a system of processes. It is more accurately referred to as the *computational algorithm* or *simulator*. It does not specifically describe an actual physical system. Rather, it consists of a set of flexible tools (i.e., a group of algorithms) for doing so. The computational model is embodied within software (i.e., a computer code such as RIP). The user of the software must provide the proper input data in order to simulate an actual physical system.

A *conceptual model* is a representation of the physical and chemical properties and processes controlling behavior of a physical system. That is, a conceptual model is essentially a body of ideas, based on available data, that summarizes the current understanding of a system. The conceptual model not only includes a description and quantification of the controlling processes and parameters, but also quantifies the uncertainties involved. (In fact, due to large uncertainties involved in geological systems, a number of *alternative conceptual models* are likely to be developed.)

The simulation model is the actual implementation of the computational model for a given conceptual model. That is, the simulation model couples the tools within the computational model (the actual computer code) with a particular conceptual model (represented by a distinct set of input data for the computer code).

Summarizing in general terms, the *computational model* is the mathematical framework embodied in the actual computer code. A *conceptual model* represents the current understanding of the physical system to be modeled. A *simulation model* is the application of the computer code using a specific data set in order to simulate the behavior of the system described by the conceptual model.

In this document, the term "model" used by itself refers only to the *computational model*. Hence, when we speak of the "radionuclide transport component model" or the "waste package component model", we are referring to the computational algorithms describing radionuclide transport pathways or waste package behavior, respectively (a component model being a subset or part of the total computational model). The complete terms "*conceptual model*" and "*simulation model*", on the other hand, are always used explicitly when referring to these two concepts.

2.2 Total System Performance Assessment Model Overview

The major portion of the RIP software is the *total system performance assessment (PA) model*. The PA model is essentially a radionuclide transport model, and consists of a series of inter-connected, fully-coupled component models. The component models consist, in general, of simple functions relating various system parameters that control processes affecting radionuclide transport. The four primary component models address:

- waste package behavior and radionuclide release;
- fluid flow and radionuclide transport in the geosphere;
- disruptive events (such as human intrusion, tectonics and volcanism) that may affect system parameters and/or processes; and
- radionuclide fate and effect (dose/risk) in the biosphere.

A schematic of the main components of the RIP PA model is shown in Figure 2-1.

Before describing in greater detail what the RIP PA model *is*, it is important to reemphasize what it *is not*. RIP *is not* a detailed deterministic model based completely on low-level physically-based parameters. (For example, it does not explicitly model radionuclide transport through the unsaturated and saturated zone by solving a three-dimensional advection-diffusion equation.) As pointed out in the previous chapter, the RIP PA model is a *descriptive probabilistic model* that *describes* rather than *explains* the system behavior and is intended to directly represent the uncertainties in processes and events and their controlling parameters. As a result, RIP relies heavily on subjective assessments of relatively high-level descriptive parameters. It is also important to note that the RIP PA model is a *preliminary* performance assessment model. It is intended to be used as a management tool to help guide site characterization, as well as a tool for project scientists who wish to carry out sensitivity analyses and/or test alternative hypotheses with respect to system performance. In its present form, it is not intended to be a licensing tool. It should be noted, however, that the structure of RIP is such that it can continually evolve, and as more details are incorporated into the model, RIP could potentially evolve into a licensing tool.

FIGURE **2-1**

RIP PERFORMANCE ASSESSMENT MODEL COMPONENTS
ARGONNE/MODEL DEVELOPMENT

2.2.1 Treatment and Propagation of Uncertainty

The purpose of the RIP PA model is to predict the future, allowing for uncertainties in our knowledge about the system being modeled, including uncertainties about the processes and future events that may occur, and uncertainties in the parameters controlling those processes and events.

As a result of these uncertainties, deterministic analysis alone is inappropriate and a probabilistic approach to performance assessment must be used. The manner in which RIP represents uncertainty in system parameters and sub-models, and how that uncertainty is propagated through the integrated PA model is discussed below. The flexible and powerful manner in which RIP handles uncertainty is a key aspect of the tool.

In order to represent the uncertainties, many of the parameters and processes related to the performance of a repository can only be represented probabilistically (e.g., by probability density functions, as opposed to single values). RIP is designed such that uncertainties in both the model parameters *and* the component models themselves can be explicitly represented. Oftentimes, performance assessment considers only parameter uncertainty and neglects model (or process) uncertainty. In complex systems, however, process uncertainty can be greater than parameter uncertainty and it must be properly represented.

There are a number of alternative approaches that could be taken to develop performance assessment predictions incorporating uncertainty:

- evaluation of the base case (a representation of the expected or most likely future for the repository system), followed by sensitivity evaluation of the ways in which the base case results would vary as a function of the uncertain parameters (e.g., "if the infiltration rate increases by X%, what will happen to the system?");
- evaluation of the base case plus a series of scenarios (i.e., alternative futures), which represent significant variants from the base case due to specific events or processes that may occur (e.g., different degrees of water-table rise, alternative types of human intrusion, alternative climates, etc.);
- sampling and simulation across the full range of potential futures randomly and repeatedly using the Monte Carlo method (i.e., repeatedly simulating the time history of repository system behavior, each time sampling the various parameter distributions describing system processes and events).

There are many variants and hybrids of the above approaches, and Appendix B compares and contrasts scenario-based approaches and simulation-based approaches.

The RIP model uses the *simulation approach*, utilizing the *Monte Carlo method* to sample the probability distributions for the uncertain parameters (describing both processes and events) and simulate a large number of system realizations in order to determine probability distributions of site performance (e.g., cumulative release, risk, transport time). That is, RIP

creates a time history of disruptive events and other system parameters for each system realization, simulates the behavior of the system under those conditions, and then combines the results of all the realizations in an appropriate manner to determine probability distributions of site performance. Because model parameters are described stochastically, each realization produces a different time history of events and processes. The integrated model is designed such that it can simulate all combinations of model parameters and time histories that might be realized within the implemented model.

An enhanced sampling scheme using both *importance-sampling* and *Latin Hypercube sampling* was developed in order to make the Monte Carlo method more efficient by improving its ability to resolve low-probability, high-consequence areas of the site performance pdfs. This scheme is discussed again in Chapter 5 and is described in some detail in Appendix C.

In general terms, the outputs from the performance assessment model consist of probabilistic performance measures for the repository system (e.g., cumulative radionuclide release to the accessible environment, maximum annual release from the waste packages, peak individual dose). That is, outputs are not single values, but distributions that specify the probability of exceedance for any particular value of the performance measures.

Figure 2-2 shows the overall logic of the RIP program, illustrating the Monte Carlo simulation approach.

2.2.2 RIP Performance Assessment Component Models

The integrated model consists of a series of fully-coupled component models. These component models consist, in general, of simple functions directly relating various system parameters in order to describe processes affecting radionuclide transport. Overall consistency is maintained by ensuring that in a given realization a parameter has a single value for all of the component models that depend on it. Correlations between sets of parameters can also be incorporated. As discussed above, the integrated model consists of four major component models:

- a model that defines and describes the performance of the waste package system (failure and radionuclide release);
- a model that defines and describes the various radionuclide transport pathways from the waste package to the accessible environment;
- a model that describes disruptive events that can directly or indirectly affect waste package performance and/or transport pathways (e.g., volcanism, human intrusion, seismic activity); and
- a model that converts concentrations in geosphere pathways (e.g., an aquifer) and/or biosphere pathways (e.g., a stream) to doses and or cancer risks to individual receptors.

FIGURE 2-2
RIP PERFORMANCE ASSESSMENT
MODEL SIMULATION LOGIC
ARGONNE/MODEL DEVELOPMENT

A schematic of the major components of the RIP PA model was presented in Figure 2-1.

The PA model incorporates radioactive decay and production of daughter products. The algorithm used to implement this is discussed in Appendix D. Additional details regarding this process are presented in the RIP User's Guide.

The *waste package behavior and radionuclide release component model* considers: 1) breaching of the waste containment system (including both container failure and dissolution and/or alteration of the waste matrix) which exposes the waste; and 2) the subsequent mass transfer of the radionuclides present within the containers to the geologic environment.

The output for the waste package component model provides input for the *transport pathways component model*, which considers transport of the radionuclides through the geosphere and/or biosphere.

The *disruptive events component model* considers the effects of discrete perturbations (e.g., earthquakes, volcanism, human intrusion) on the behavior of the other PA model components. That is, disruptive events could potentially change the behavior of the containment system (e.g., waste packages could be instantaneously disrupted or moved), or modify the behavior of the geologic transport pathways (e.g., a new transport pathway could be created or the properties of an existing pathway could be modified).

The *dose/risk component model* converts concentrations in geosphere and/or biosphere pathways to doses (or risks) to exposed individuals (receptors). Conversion factors are defined by the user.

The RIP structure for each component model was designed from the top down, starting with a broad description of processes of interest. The software is designed such that the user can increase the amount of detail and complexity in nearly any portion of the component models. That is, through a method of encapsulation, the component models can themselves be made up of sub-components.

For example, the waste package model contains sub-models for corrosion of the outer and inner barriers, alteration/dissolution of the waste matrix, and radionuclide transport in the near field. The user might elect to define subsidiary lower-level models to support the sub-models. For example, the user could define a model of the chemical evolution of the near-field environment. The encapsulation process may proceed to an arbitrary depth, but is limited in complexity by the necessity for the calculations to be extremely rapid (to facilitate efficient use of the Monte Carlo method).

Sub-models range from simple analytical expressions to more complex numerical subroutines. Some sub-models (and parameters) are time-dependent. That is, as shown in Figure 2-2, the integrated model essentially "time-steps" through the simulations, taking into account the time-dependent parameters affecting the waste package source term and other system parameters, as well as radionuclide decay chains. For example, corrosion processes could have a sensitivity to the time-varying thermal, chemical and moisture conditions near the waste packages.

In the interest of computational efficiency (which is necessary for probabilistic analysis), the component models built into RIP are greatly simplified compared to state-of-the-art process models. Where appropriate, the increased uncertainty caused by such simplification can be reflected in parameters describing *model uncertainty*. This explicit representation of model uncertainty is important for two reasons: 1) it provides a more accurate representation of the true overall uncertainty; and 2) it allows evaluation of the potential benefits of development of better models. Model uncertainty could be incorporated into a model by the user in a number of ways, such as 1) defining a stochastic parameter (e.g., normal about 1.0) which explicitly modifies a computed value to account for process uncertainty; or 2) assigning a probability to a particular process (e.g., specifying a probability that colloidal transport will be active in a particular pathway).

It is important to emphasize that although it is currently unfeasible to use detailed low level models directly for probabilistic analysis, it is possible to use these models indirectly. That is, it is intended that the high-level parameters for the component models within RIP should be based, when possible, on the results of these detailed models. For example, a detailed model could be run externally a number of times to create a response surface or an analytical expression that could then be used to describe the dependencies of a high-level parameter within RIP.

The basic concepts of the four major components models (waste package behavior and radionuclide release, radionuclide transport pathways, disruptive events, and dose/risk) are summarized in the following sections. These components are discussed in detail in Chapters 3, 4, 5, and 6.

2.2.2.1 Waste Package Behavior and Radionuclide Release Component Model

The waste package model is described in detail in Chapter 3. A brief summary of its capabilities is provided in outline form below.

General Model Structure

- The waste package component model is part of the total system performance model, and is directly coupled to component models describing disruptive events and radionuclide transport pathways.
- The model is based on subjective assessments of relatively high level phenomenological parameters, such as container and cladding/pour canister failure distributions, and generalized alteration and mass transfer parameters.
- The model simulates groups of waste packages (rather than tracking the behavior of each of the individual waste packages in the repository).
- Waste package parameters can be described by the user as a function of temporally varying environmental conditions.

- The model incorporates radioactive decay and production of daughter products.

Environmental Conditions

- Temperature and moisture conditions are explicitly included in the model. The temperature at the edge of the waste package varies with time. Moisture conditions refer to the mode of water contact at a waste package (which are completely user-defined). Both temperature and moisture conditions can be specified as variable across the repository.
- Other environmental conditions (e.g., chemistry, stress) can be added by the user. Environmental conditions can be described as being spatially and temporally variable.
- A simple rewetting model is used that assumes that waste packages return to specified moisture conditions upon reaching a specified temperature. At temperatures above the specified temperature, the waste package is considered to be dry.

Waste Package Failure Rates

- Two levels of waste package containment (and failure) are explicitly simulated: the primary container (the waste package itself); and the secondary container (e.g., cladding for spent fuel, pour canisters for high level defense waste).
- Waste package failures are described in terms of density functions of failure frequency.
- Containers and cladding/pour canisters can fail by one or more failure modes. The model combines failure modes by assuming that the failures can be treated independently (they do not act with synergism).
- Container failure modes can be affected by temporally varying environmental conditions.

Mass Exposure

- Exposure of radionuclides is brought about by primary and secondary container failure, as well as matrix alteration/dissolution processes.
- The radionuclide inventory is made up of three additive components: the free inventory, which is exposed immediately upon primary container failure, the gap inventory, which is exposed immediately upon secondary container (e.g., cladding) failure in a failed container, and the bound inventory, whose exposure is controlled by alteration/dissolution of the waste matrix.
- Exposure of the bound inventory can be controlled by dissolution of the matrix and/or air alteration of the matrix. Dissolution is described in terms of a matrix

dissolution rate and an effective wetted surface area. Dissolution is zero prior to rewetting of the waste package.

- The effective wetted surface area of matrix can be described as a function of container failure mode. It is assumed that for a waste package that fails by more than one mode, the effects on wetted surface area are additive.

Mass Transfer

- For an aqueous radionuclide, mass transfer can be described as an advectively or a diffusively controlled process, each of which may be limited by radionuclide solubilities.
- Aqueous mass transfer is set equal to zero prior to rewetting of the waste package.
- Diffusive mass transfer can only be described in the waste package component model as a steady state process. The pathways component model can be appropriately used, however, to represent transient diffusive releases.
- Several mass transfer parameters can be described as functions of container failure mode. It is assumed that for a waste package that fails by more than one mode, the effects on mass transfer are additive.
- The mass transfer rate for gaseous species is directly specified by the user.

Effect of Disruptive Events

- Disruptive events can affect the behavior of the waste package. Disruptive events are simulated in a separate model component. Their consequences can manifest themselves in the waste package model in three ways: 1) a portion of the waste packages can be disrupted in place; 2) a portion of the waste packages (and their inventory) can be moved directly to the accessible environment or some other location; and 3) the parameters describing waste package behavior and/or environmental conditions may be changed.

Linkage to Transport Pathways Model

- The waste package model is coupled with the transport pathways model in two ways: 1) it relies upon the same large scale hydrologic parameters utilized and/or defined within the transport pathways component (e.g. repository level flow rate); and 2) each waste package type discharges its mass to a specified transport pathway (or pathways) defined by the user.

2.2.2.2 Radionuclide Transport Pathways Component Model

The pathways model is described in detail in Chapter 4. A brief summary of its capabilities is presented below.

The task faced by the RIP pathways model is to probabilistically simulate radionuclide transport through the geosphere. Knowing that continuum-based models cannot be practically used for this task, the RIP model algorithm was designed in a different way. The near and far field radionuclide transport algorithm for the RIP model is based on a network of user defined pathways. The pathways of RIP reflect major features of the hydrologic system and the biosphere, and are conduits through which transport occurs. In a RIP application, the user sets up a pathway "network" relevant to what is known about the system. The pathways may be used for both flow balance and radionuclide transport purposes. They may account for either gas or liquid phase transport.

The purpose of a pathway is to represent a homogeneous region within the large scale heterogeneity of the hydrologic system or biosphere, such as geologic structures, formation scale stratigraphy, ponds, streams or the atmosphere. In a simple homogeneous system, only a single pathway may be necessary. In highly complex systems (such as Yucca Mountain) up to 30 pathways are likely to be required in order to account for the large scale heterogeneity.

RIP geosphere pathways are characterized by flow modes, which address heterogeneity at the local scale. For example, flow in rock matrix and flow in fractures may be two interacting flow modes within a single pathway. The flow modes are primarily distinguished from one another based on flow velocity in the mode. However, retardation parameters and the proportion of the total pathway flow may also be different from one flow mode to another.

The actual transport of radionuclides along a geosphere pathway is based on a breakthrough curve. In RIP, the breakthrough curve is developed as a cumulative probability distribution for radionuclide travel times along the pathway. The probability gives the expected proportion of radionuclides that would have traversed the pathway by a specified time, which is equivalent to a breakthrough curve. The breakthrough curve for a pathway combines the effects of all flow modes and retardation on the radionuclide travel time. It is developed based on a Markov process algorithm, which is similar to a random walk through the flow modes.

The RIP pathways model incorporates a number of simplifying approximations made in the interest of reducing computer run times. Nevertheless, it is a very flexible and adequately accurate approach for stochastic modeling.

As can be seen even from the brief description provided above, the RIP pathways model is significantly different from other models that have typically been applied to groundwater flow and radionuclide transport at proposed repository sites. The reason for this is the authors' observation that available models, while representing portions of an overall system well, *often fail to capture the essence of the overall hydrogeologic system*. For example, one-dimensional models cannot capture effects such as fingering, perching, and diversion to faults. Even three-dimensional models do not capture all the important aspects of a fracture system, and do not have adequate spatial resolution to accurately simulate small-scale behavior such as fracture termination and matrix-block imbibition. None of the available models adequately represents coupled water/vapor/air flow in the unsaturated zone (critical for an unsaturated site such as Yucca Mountain).

The absence of adequate models is revealed most tellingly by considering, as an example, the following observation regarding the US DOE's Yucca Mountain site: *at the present time, there is no valid water-balance model that explains the flow of water at the Yucca Mountain site, and predicts results consistent with observed field data.*

The RIP authors have tried to develop a model capable of representing and determining the implications of what is known about a site *at the present time* (which in many cases is very little). Thus, the RIP model is based on a phenomenological approach that attempts to *describe* rather than *explain* the system.

While project scientists may not yet have adequate data and models to develop a full mathematical model of a particular site, they typically have a good understanding of the kinds of processes that can occur there, both now and in the future. The RIP pathways model was specifically developed to describe this type of situation. While many of the necessary input data for a study may originally be little more than educated guesses based on limited data and physical bounds, the idea is that further data collection efforts and more advanced low-level modeling will produce significantly better (and more defensible) input data at some time in the future. As has been pointed out, one of the primary purposes of RIP is to evaluate what types of data and models will be most valuable.

2.2.2.3 Disruptive Events Component Model

The disruptive events model is described in detail in Chapter 5. A brief summary of its capabilities is presented below.

Disruptive events are defined here as discrete perturbations of the repository system. That is, disruptive events are discrete occurrences that have some quantifiable effect on the processes described by the other two component models. Note that discrete is a relative term, and does not necessarily imply instantaneous. Given the long time scales of interest (10,000 years or more), something taking place over a period of 100 years could be considered a discrete event. Examples of disruptive events under this definition include volcanism, faulting, and human intrusion. In general, the disruptive events component model is intended to represent relatively rare occurrences. Events that occur continuously throughout the time period of interest are more efficiently modeled as processes within the other component models.

Climate change would generally not be treated as a disruptive event, since this is a process that occurs gradually, and some sort of climate change is expected in the future (although the actual nature of the change is uncertain). Climate change (and the corresponding changes in environmental conditions such as water table elevation and infiltration rate) can be treated explicitly in the transport pathways and waste package behavior components.

The *occurrence* of disruptive events is described as follows:

- RIP requires input by the user describing all *significant events*: events that are both credible and consequential.

- Each significant event must be assigned an annual rate of occurrence, λ . It is also necessary to specify whether an event can reoccur. In addition, each disruptive event can be assigned one or more *descriptor parameters*. Descriptor parameters define the characteristics and magnitude of the event. For example, the descriptor parameters for a human intrusion/drilling disruptive event might be the number of boreholes drilled, and the deepest pathway (i.e., formation) intersected.
- Event occurrences are simulated as Poisson processes.

For each disruptive event, there are four types of internally-defined disruptive event *consequences* that describe possible discrete responses of the system:

- The radionuclides in a number of waste packages are moved directly to the accessible environment. It is assumed that the inventory released from each package is equal to the inventory of an unfailed container at the time of the event.
- The radionuclides in a number of waste packages are moved directly to a specified pathway (e.g., the saturated zone). It is assumed that the inventory released from each package is equal to the inventory of an unfailed container at the time of the event. It is also assumed that all of the waste package's inventory is immediately released to the pathway (i.e., the waste package is completely disrupted during the movement and the contents are not limited by any alteration, dissolution, or mass transfer processes at the waste package).
- A number of waste packages are disrupted in place.
- A portion of the mass (previously released from the waste packages) contained within a pathway is immediately discharged to the accessible environment.

In addition to the four *discrete consequences* described above, which are explicitly included in the model, it is also possible to directly influence parameters defined in the waste package, transport pathway, and dose/risk modules, and this capability can be used to specify *long-term consequences*.

2.2.2.4 Dose/Risk Component Model

The dose/risk model is described in detail in Chapter 6. A brief summary of its capabilities is presented below.

Doses are computed as a function of *concentrations* present in some environmental media (e.g., soil, groundwater, surface water). Environmental media can be represented in RIP in two ways: 1) by geosphere pathways, such as a water supply aquifer; and 2) by biosphere pathways (also called biocells), such as a stream. The RIP pathways component model keeps track of radionuclide mass as it moves through the geosphere/biosphere system.

In a geosphere pathway, mass is transported based on a breakthrough curve (as mentioned in Section 2.2.2.2). Concentrations are computed based on the mass in a pathway, and the pathway's dimensions, porosity and sorption properties. In a biosphere pathway, mass is transported based on a specified turnover rate. Concentrations are computed based on the mass in the pathway and a specified pathway volume.

The dose to a user-specified *receptor* from a particular radionuclide is computed as the sum over all pathways through which the receptor is exposed of the product of the pathway's concentration and an appropriate *dose conversion factor*. The dose conversion factor is defined as the dose received from a unit concentration of radionuclide in a given environmental medium (e.g., water from an aquifer; water from a river; contaminated soil). The dose conversion factor is directly specified by the user. It is nuclide-specific and dependent on a number of factors that determine the amount of exposure (e.g., amount of water consumed, amount of water used for irrigation, etc.).

Doses can be converted to the lifetime incremental cancer risk to a member of the receptor group by multiplying by a linear *risk factor*.

2.2.3 Performance Assessment Model Input and Output

RIP is designed with an interactive menu-driven user-interface that allows the user to easily enter input parameters. The specific types of input parameters required by each component model are discussed in detail in the following chapters. The RIP User's Guide describes the user-interface in detail. The user-interface, which allows enormous flexibility in specifying input parameters, is also discussed in general terms below in Section 2.4.

The RIP user-interface is also designed to allow the user to specify and manipulate the output and present it in a variety of forms. The specific forms of the output are discussed in general terms in subsequent sections of this document and in detail in the RIP User's Guide.

As discussed above, the output for RIP consists of performance measures for the repository system. These performance measures are probabilistic in nature. That is, output is not a single value, but a distribution that specifies the probability of exceedance for any particular value for the performance measure.

It is worthwhile to briefly discuss here the ways in which the probabilistic results generated by RIP are presented. As an example, we will consider one of the probabilistic performance measures that can be output by RIP: the cumulative release of radionuclides to the accessible environment (e.g., over a 10,000 year period).

Recall that the Monte Carlo method utilized by RIP will essentially simulate a large number of system realizations. Each realization will produce a single value for cumulative release. Each individual result will be weighted in a manner that reflects how the realizations were sampled. For example, if realizations are sampled in a totally random manner, each result will have an equal weight; if realizations were sampled in a biased manner (as described in Appendix C), results would have different weights.

The simplest way in which to display these results would be in the form of a probability density function (pdf). In simple terms, this plots the frequency of the various cumulative release results, and is illustrated schematically in Figure 2-3a. A probability density function is seldom suitable for presenting Monte Carlo results due to the discrete form of the results, which produces "jagged" probability densities.

An alternative manner of presenting the same information is the cumulative distribution function (cdf). This is formed by integrating over the pdf and is illustrated schematically in Figure 2-3b. By definition, the total area under the pdf must integrate to 1.0, and the cdf therefore ranges from 0.0 to 1.0. As shown in the figure, a particular point, say $[r_i, p_1]$, on the cdf is interpreted as follows: p_1 = the probability that the cumulative release is *less* than r_i .

The final (and most common) manner of presenting this information is the complementary cumulative distribution function (ccdf). The ccdf is illustrated schematically in Figure 2-3c. As shown in the figure, a particular point, say $[r_i, p_2]$, on the ccdf is interpreted as follows: p_2 = the probability that the cumulative release is *greater* than r_i . Note that the ccdf is the complement of the cdf. That is, $p_2 = 1 - p_1$.

In addition to presenting probabilistic results in the three manners outlined above, RIP can also manipulate the output data in order to carry out detailed *sensitivity analyses*. Note that for each individual realization, RIP not only saves the performance result, but also saves all of the input parameters. This allows the user to carry out a variety of post-processing exercises to examine the sensitivity of the performance results to specific model parameters or groups of parameters.

2.2.4 Results Post-Processing

A RIP analysis can typically involve hundreds of independent stochastic parameters, and numerous performance measures may be calculated. The results of several thousand realizations of such an analysis would be very difficult to interpret without good analytical tools. Therefore, RIP has a post-processing module that assists the user in making sense of the results, and identifying the most significant parameters and the way in which they affect the system performance.

The post-processing module in RIP allows the user to review and analyze the results of the Monte Carlo simulations. The post-processing is primarily graphical or statistical analyses of how the system results are affected by different input parameters.

The user takes the following three steps in post-processing:

- he selects which result he is interested in (e.g., a time-history of radionuclide release, or a waste package failure rate, etc.),
- he selects a subset of the results (e.g., all results, or the worst 5% of results, etc.)
- he selects the type of analysis to perform.

a) Probability density function

b) Cumulative distribution function

c) Complementary cumulative distribution function

FIGURE 2-3
PRESENTATION OF
PROBABILISTIC RESULTS
ARGONNE/MODEL DEVELOPMENT

There are a number of options for each of the above steps. For example, the user can select a subset of results based on how the system performed (e.g., the 'bad' results), or on the value of some input parameter (e.g., all results involving human intrusion), or both. Similarly, a variety of analyses may be performed, including the following:

- direct display of the inputs and results for the Monte Carlo realizations;
- a display of correlations between results and input parameters;
- a scatter plot of the result versus an input parameter;
- a 3-d plot of the result as a function of two input parameters;
- a display of time-histories of selected results from particular 'bad' realizations.

These post-processing functions are intended to assist the user in developing an understanding of which combinations or ranges of input parameters result in better or worse performance of the repository system.

RIP also provides the option to write results to an output file in a format compatible with commercially available statistical analysis software packages, allowing more complex sensitivity analyses to be carried out.

An additional method of post-processing analysis, strategy modeling, is described briefly in the next section, and in detail in Chapter 7. Strategy analysis allows the RIP user to evaluate the likely results of new information (from site characterization activities) in terms of changes in the confidence of performance predictions.

The results post-processor for RIP is discussed in detail in the RIP User's Guide.

2.3 Strategy Evaluation Model Overview

As described previously, the performance assessment model is embedded within a decision analysis model that allows the user to evaluate alternative site characterization strategies, where a strategy is defined as a group of activities. Figure 2-4 provides a schematic of the RIP strategy evaluation model. As discussed in Chapter 1, the RIP strategy model provides three outputs by which alternative strategies can be evaluated:

- a probabilistic estimate of cost;
- a probabilistic estimate of duration; and
- a probabilistic evaluation of the predicted site performance resulting from implementation of the strategy.

FIGURE 2-4
OVERVIEW OF RIP
STRATEGY EVALUATION
ARGONNE/MODEL DEVELOPMENT

Computation of the first two (probabilistic cost and duration) is straightforward. Computation of the third, the probabilistic reduction in performance assessment uncertainty, is relatively novel and complex and is discussed briefly here.

Given a current data set of system parameters, and information describing how parameter uncertainty will be reduced by a given characterization strategy, RIP realizes a set of *post-strategy system parameter distributions*. That is, the current data set (in particular, the uncertainty in specified system parameters) is modified to reflect the effects of carrying out the activities within a characterization strategy. This modification is carried out using a Bayesian updating algorithm. Because we can not predict precisely how a parameter's distribution will change due to an activity, but can only estimate how the *magnitude of the uncertainty* will be affected (i.e., the distribution shape may narrow, but we can't predict whether it will shift up or down), the results of a particular strategy can only be described probabilistically. Figure 2-5 shows how the probability distribution for one particular parameter might change as a result of carrying out a strategy. (In this example, it has been assumed that the characterization strategy will reduce the parameter uncertainty by a factor of three.) In effect, a particular strategy defines a *probability distribution of sets of resulting system parameter distributions*. The RIP strategy model samples this distribution of sets many times.

Based on the parameter distributions within a given realized set, RIP uses the performance model to produce a probabilistic evaluation of repository performance measures. As illustrated in Figure 2-6, each realized set of parameter distributions produces unique probabilistic performance results (e.g., in the form of a CCDF of cumulative release). By realizing many different sets of parameter distributions for a particular strategy, producing a probabilistic performance result for each, and combining this suite of results in an appropriate manner, it is possible to determine probabilistically how that particular strategy is likely to affect the evaluation of site suitability.

In practice, the algorithm used in RIP is somewhat simpler than that indicated in Figure 2-4. It is not actually necessary to re-run the performance model each time the updated probability distributions are produced by simulating a strategy. In fact, it is only necessary to run one full set of performance model analyses. Subsequently, the relative probabilities of each realization can be modified based on the updated probabilities for the parameters to create the revised performance probability distributions (such as those shown in Figure 2-6).

An example of how this can be carried out is schematically illustrated in Figure 2-7. In this example, the post-strategy probability distribution of a performance result for a particular value of a performance measure ($R = 10$) is plotted (i.e., a vertical slice through Figure 2-6 at $R = 10$). Strategy A is the same strategy shown in Figure 2-6. Strategy B is an alternative strategy. This figure indicates that very little knowledge regarding system performance will be gained by carrying out strategy B, while strategy A is likely to greatly change the current performance prediction. Note the asymmetric nature of the post-strategy distributions, indicating that the provision of additional information is most likely to move the distribution towards the expected value. That is, although there is always the possibility of a bad surprise (i.e., predicted performance is worse), the expected result of a strategy is to bring the tails of the distribution inwards toward the prior mean (this is precisely what reducing uncertainty means).

FIGURE 2-5
 UPDATING THE PROBABILITY DISTRIBUTION
 FOR A SINGLE SYSTEM PARAMETER
 ARGONNE/MODEL DEVELOPMENT

FIGURE 2-6
 SUITE OF PERFORMANCE
 RESULTS FOR STRATEGY A
 ARGONNE/MODEL DEVELOPMENT

FIGURE 2-7
PROBABILITY OF POST-STRATEGY
PERFORMANCE RESULTS
ARGONNE/MODEL DEVELOPMENT

The strategy evaluation model is described in detail in Chapter 7.

2.4 Parameter Definition and the Flexibility of the RIP Software

Throughout this report reference will be made to 'input parameters' for RIP. While certain types of input parameters are explicitly required by RIP, the software contains logic that allows the user to define additional parameters and equations for very general kinds of system components. That is, the model consists of a basic computational framework representing the controlling processes, but is intentionally flexible such that the user can represent the processes with as much detail as desired.

The user can even create and specify processes and parameters that are not explicitly incorporated into RIP. In a sense, the RIP program is similar to a spreadsheet: while it contains a large amount of built-in logic and calculational capabilities, the problem that is solved is entirely defined by the user. That is, RIP has been developed such that it is relatively free of assumptions regarding the details of waste package behavior and radionuclide transport processes. Similarly to a spreadsheet user, the RIP user can define a very simple model, or a very complex one. RIP can be run on a personal computer, for simple problems, or can be linked to a powerful workstation for solving more complex ones. The reader of this report who may be daunted by some of the theory described in later chapters should not abandon hope: it is possible to use RIP in a relatively simple manner to address relatively simple, though perhaps very important, issues.

The cornerstone of the RIP methodology, which it is critical to understand in order to take full advantage of the software, is the concept that model input parameters can be defined by the user with a great deal of flexibility. In particular, *a given system parameter can be specified as a constant, a stochastic (i.e., represented as a probability distribution), or as a function of other parameters* (which themselves can be constants, stochastics, or functions).

Representing system parameters as *stochastics* allows the RIP user to specify the degree of *uncertainty* in a particular parameter. For example, if the current level of knowledge regarding a particular system parameter (such as an elemental solubility) is such that it is only possible to specify its value within certain limits (e.g., greater than 10^{-4} g/m³ but less than 10^{-1} g/m³), it would be most appropriate to specify this parameter as a probability distribution (e.g., a log-uniform distribution ranging between 10^{-4} and 10^{-1}). RIP allows the user to choose from a wide variety of probability distributions (e.g., normal, log-normal, triangular, beta, gamma, discrete, etc.) for a stochastic parameter. For each Monte Carlo realization of the repository system, all of the stochastic parameters are sampled from their specified distributions.

The ability to represent system parameters as *functions* of other parameters imparts to the user the ability to readily add detail to any given system parameter or process represented by RIP. The user interface of the software is designed such that the user literally types in the desired function. In addition to standard mathematical operators (e.g., SIN, COS, MAX, ERF, LOG), the user can define functions using relational operators (e.g., >, <, =) and IF, THEN logic. Such flexibility allows the user to easily modify and add detail to the conceptual and computational

model *without having to make changes to the software* (i.e., without modifying and compiling the source code).

As an example, suppose that instead of representing an elemental solubility as a stochastic parameter (as illustrated above), the user wished to incorporate a solubility model that explicitly accounted for the effects of temporally or spatially variable chemistry (e.g., pH) conditions. To accomplish this, the user could define a new parameter, called *pH*. This parameter could be defined as a constant, a stochastic, or a function (of other parameters or of time). It could also be assigned a random spatial variability throughout the repository. The elemental solubility could then be described as a function of this parameter. For example:

$$\text{SOL}_n = (A \times \text{pH}) + B \quad (2.1)$$

where SOL_n is the solubility of element *n* and *A* and *B* are constants or additional user-defined parameters.

For more complex functions, the software is structured such that the user can develop separate coded functions (i.e., separate coded program modules, written in the C programming language) which can then be directly coupled with the main RIP algorithms.

Note also that the concepts of stochastics and functions can be combined. For example, the solubility of a species could be defined as a log-normal distribution whose mean and standard deviation were functions of pH.

Use of the *Parameters Module*, the software component that implements the concepts described above, is discussed in detail in the RIP User's Guide.

2.5 Summary of the Repository Integration Program

RIP is a powerful and flexible computational tool for carrying out probabilistic integrated total system performance assessments for geologic repositories. It embodies probabilistic decision analysis tools that allow it to:

- examine parameter sensitivity;
- evaluate alternative conceptual designs; and
- evaluate alternative site characterization strategies.

The primary purpose of RIP is to provide a management tool for guiding system design and site characterization. In addition, the performance assessment model (and the process of eliciting model input) can act as a mechanism for integrating the large amount of available information about a repository into a meaningful whole (in a sense, allowing one to keep the "big picture" and the ultimate aims of the project clearly in focus). Such an integration would be useful both for project managers and project scientists.

RIP is based on a "top down" approach to performance assessment which concentrates on the integration of the entire system, and utilizes relatively high-level descriptive models and parameters. The key point in the application of such a "top down" approach is that the simplified models and associated high-level parameters must incorporate an accurate representation of their uncertainty.

RIP is designed in a very flexible manner such that details can be readily added to various components of the model without modifying the computer code. Uncertainty is also handled in a very flexible manner, and both parameter and model (process) uncertainty can be explicitly considered. Uncertainty is propagated through the integrated PA model using an enhanced Monte Carlo method.

RIP must rely heavily on subjective assessment (expert opinion) for much of its input. The process of eliciting the high-level input parameters required for RIP is critical to its successful application. As a result, in order for any project to successfully apply a tool such as RIP, an enormous amount of communication and cooperation must exist between the data collectors, the process modelers, and the performance assessment modelers. This is because such a tool must constantly evolve and is only valid for decision making when it actually incorporates the *current state of knowledge*. This is only possible if project scientists *think in terms of performance assessment*, at least to the extent that their results can be readily incorporated into a total system model. In effect, they must be familiar with that portion of the total system performance assessment model that represents the particular process or parameter that they are studying, such that they can recommend modifications in the data (or the model itself if necessary) as more information becomes available. Without this type of integration between the performance assessment modelers and the project scientists, a tool such as RIP can not be validly applied.

The details of the RIP algorithms are described in the remaining chapters. Chapters 3, 4, 5, and 6 describe the four components of the performance assessment model, and Chapter 7 discusses the strategy evaluation model in which the PA model can be embedded.

3. WASTE PACKAGE BEHAVIOR AND RADIONUCLIDE RELEASE MODEL

3.1 Introduction

As discussed in Chapter 2, the RIP integrated repository performance assessment model is a complex radionuclide transport model, and consists primarily of a series of inter-connected, fully coupled component models with input/output relationships for radionuclide transfer. The four major component models address waste package behavior and radionuclide release, transport pathways to the accessible environment, disruptive events, and fate and effect (dose/risk) in the biosphere.

The purpose of this chapter is to describe the structure of the integrated performance assessment model's waste package behavior and radionuclide release component model. The general methodology and assumptions incorporated into the software are presented in detail, and application of the model is discussed. The waste package component model discussed below includes both the waste package itself and the engineered barrier system (EBS).

Considerable effort and progress has been made at developing performance assessment tools for the waste package and the EBS over the last several years (more so than in other areas of repository performance modeling, such as unsaturated zone radionuclide transport), and several models have been developed and are continuing to be revised (e.g., Liebetrau et al., 1987; O'Connell, 1990; Robinson and Worgan, 1991). The waste package model within RIP relies upon some of the same basic concepts employed by these existing codes.

RIP is primarily distinguished by its unique "parameters module" (described briefly in Chapter 2 and in detail in the RIP User's Guide) and user-interface that make the software enormously flexible as well as powerful, allowing the user to easily define new model parameters and create alternative conceptual models of waste package behavior. Uncertainty and variability can easily be incorporated by the user into any model parameter that has been defined. Furthermore, because RIP is an integrated total system performance model, of which the waste package model described here is but one component, waste package behavior is directly coupled with component models describing disruptive events and radionuclide transport through the geological environment. This allows waste package parameters and processes to be directly analyzed with respect to *total system performance*.

These features are important, because in addition to acting as a management tool, it is intended that RIP can become a valuable tool to project scientists who wish to carry out sensitivity analyses and/or test alternative hypotheses with respect to total system performance. The software was specifically designed to facilitate such analyses.

It is intended that existing lower-level (i.e., more detailed) waste package models eventually be used to provide input for RIP and/or as benchmarks during model validation exercises.

3.1.1 Chapter Organization

The RIP waste package behavior and radionuclide transport model is described in detail in the following sections. Section 3.2 presents the general methodology for computing radionuclide release from waste packages. Section 3.3 then describes how near-field environmental conditions (and variability in these conditions) are superimposed on this methodology. Section 3.4 presents a general discussion of the required input parameters and the form of the model output. Section 3.5 provides a general schematic summary of the model, and also reiterates the inherent assumptions on which the computational structure is based. This is critical as model results must always be viewed with a full understanding of the assumptions and limitations of the computational algorithm and the input data. To assist the reader, a list of symbols (and their definitions) that are used is included in Section 3.6.

3.2 General Algorithm for Waste Package Behavior and Radionuclide Release

The purpose of the waste package behavior and radionuclide release model is to generate a time history of release from the emplaced waste packages for each radionuclide. To accomplish this, the waste package behavior model must consider two types of processes: 1) breaching of the waste containment system itself (in the case of spent fuel waste, container and cladding) which exposes the waste; and 2) the subsequent mass transfer of the radionuclides present within the containers to the geological environment. These processes are dependent on environmental conditions. Figure 3-1 is a schematic of the waste package release processes (in this case, for an unsaturated repository). As shown in this figure, both exposure of the waste, as well as mass transfer of the radionuclides, are dependent on environmental conditions. The model explicitly considers the influence of environmental conditions, such as moisture and temperature (including modeling a "thermal period" during which waste packages may be dried out upon heating and subsequently rewet upon cooling.)

Due to the complexity of the processes controlling waste package behavior, it is generally agreed that it is not presently possible to build a practical waste package behavior model based on low level physical parameters and first principles (Golder Associates, 1991). As pointed out in Chapter 1, a more realistic approach is to build a model based on subjective assessments of relatively high-level phenomenological parameters. In particular, the waste package model described below is built primarily upon two types of high-level parameters: those describing primary and secondary container failure distributions (which determine when and what portion of the waste inventory is exposed), and those describing radionuclide exposure and mass transfer.

Consistent with this approach, the model has been developed such that it is relatively free of assumptions regarding the details of waste package failure, mass exposure, and mass transfer processes. That is, the model consists of a basic computational framework representing these controlling processes, but is intentionally flexible such that the user can represent the processes with as much detail as desired. For example, a model parameter (such as the matrix alteration rate), can be described by the user not only as a constant or a stochastic (i.e., uncertain) variable, but if necessary, as a complex function of other defined model parameters. As described in Chapter 2, the user interface of the software is designed such that the user literally types in the

mass release rate = f(mass exposure, mass transfer)
 mass exposure, mass transfer = f(environmental conditions)
 environmental conditions = moisture, temperature, chemistry...

(after Apted et al. 1991)

FIGURE 3-1
WASTE PACKAGE SCHEMATIC
 ARGONNE/MODEL DEVELOPMENT

desired function. This allows the conceptual model of waste package behavior to be continuously and easily modified as more information becomes available (without modifying the RIP computer code). The user interface is described in detail in the RIP User's Guide.

The waste package behavior algorithm described here is deterministic. That is, it simulates a single system realization. However, as pointed out previously, uncertainty in both the model parameters and the component models themselves is explicitly included in the integrated stochastic model. Due to the inherent uncertainties resulting from our lack of knowledge, many of the parameters will be represented by probability density functions (pdfs). The integrated model uses a modified Monte Carlo method to sample these distributions and simulate a large number of random system realizations (using the deterministic model) in order to determine probability distributions of site performance (e.g., cumulative release, transport time).

Both parameter *uncertainty* and parameter *variability* can be explicitly represented in the waste package model. *Uncertainty* in a model parameter implies a lack of knowledge regarding the actual value of that parameter. This is represented in the model by describing the uncertain parameter as being stochastic (i.e., represented as a distribution). The parameter's distribution is randomly sampled each realization. That single parameter value is then used throughout the realization.

Variability in a model parameter implies that for a given realization, a distribution of parameter values exists. An example of a variable parameter would be one that describes water contact modes at a waste package. Due to hydrogeological variability, one would expect the mode of water contact to vary from waste package to waste package throughout the repository.

In the model, variability is represented by discretizing the repository into groups of waste packages, and summing the contributions from these groups. The waste packages within a given group are assumed to be under similar environmental conditions, which vary from group to group. These groups are defined based on a number of environmental factors (such as water contact mode) whose variability is considered to be significant. The use of groups has important implications with respect to the capabilities and limitations of the model and will be discussed further in subsequent sections.

It should be noted that although the waste package computational algorithm discussed below is based on high-level phenomenological parameters, the reader will find that it is still fairly complex, and includes a variety of options that enable more detailed representation of various processes. This complexity was unavoidable in order to ensure that the software is able to realistically represent critical aspects of waste package behavior and radionuclide release. Nevertheless, it is important for the reader to realize that the complexity of the waste package model is completely controlled by the user. That is, due to the flexibility of the user-interface, the user can quickly define a very simple (and approximate) waste package model, or, alternatively, can take more time and effort and define a very detailed waste package model. This flexibility may be difficult to fully appreciate prior to reading the user's guide and actually using the software directly.

The general methodology for developing the failure distributions and using them in combination with radionuclide inventories, dissolution rates, and mass transfer rates to generate

waste package release rates for each radionuclide is discussed in detail below. Representation and incorporation of near-field environmental conditions is discussed in Section 3.3, and a summary of model input parameters is provided in Section 3.4.

3.2.1 Overview of Radionuclide Release Calculation

In order for radionuclides to be released from a waste package, they must first be exposed to the near field environment. This is brought about as a result of waste package failure and subsequent waste matrix alteration/dissolution. Even after a given mass of radionuclide is exposed, however, it is not considered to be released until the mass is physically transferred away from the immediate vicinity of the waste package (e.g., a low solubility constituent may be exposed but never released). This transfer occurs via advective and diffusive processes, and is described in the RIP model by parameters defining the rate of mass transfer. Figure 3-2 summarizes the radionuclide release calculation.

The instantaneous release rate for a given radionuclide is dependent on both the rate at which mass is exposed to the near field environment and the maximum rate at which mass can be transferred out of and away from the waste package. In general, the slower of these two rates is the rate-limiting process defining the actual release rate. Because these two rates may vary temporally, however, this generalized rule is not strictly correct.

Consider, for example, a situation in which the mass transfer rate is initially much smaller than the exposure rate. Under these conditions, the release rate is controlled by the mass transfer rate. As a result, exposed mass "accumulates" at the waste package (since mass is being exposed faster than it is being transferred away). Imagine now that the exposure rate eventually drops below the maximum possible rate of mass transfer (e.g., due to a change in environmental conditions or exhaustion of the supply of unexposed mass). Under these conditions, it is incorrect to assume that the release rate is controlled by the slower of the two rates (the exposure rate), since a quantity of mass (exposed previously) is still available to be released.

It is therefore apparent that the instantaneous release rate is not only dependent on the rate of exposure and rate of mass transfer, but is also dependent on the amount of available (i.e., previously exposed) mass still present in the immediate vicinity of the waste package. The actual calculation of the release rate as a function of these three parameters is shown below.

FIGURE 3-2
OVERVIEW OF WASTE
PACKAGE BEHAVIOR MODEL
ARGONNE/MODEL DEVELOPMENT

Let:

- $r(n,t)$ = the release rate of radionuclide n from the waste package at time t [M/t];
- $e(n,t)$ = the rate at which radionuclide n within the waste package is being exposed to the near field environment at time t (a function of the waste package failure and matrix alteration/dissolution rates) [M/t];
- $k_i(n,t)$ = the maximum possible mass transfer rate of radionuclide n out of and away from the waste package at time t [M/t];
- $M(n,t)$ = the amount of exposed (available) mass of radionuclide n at the waste package at time t [M]; and
- Δt = the computational time step for simulation [t].

Given these definitions,

$$M(n,t) = \int_0^t [e(n,\tau) - r(n,\tau)] d\tau \quad (3.1)$$

The release rate, $r(n,t)$, is determined as follows:

- if $M(n,t) = 0$,
then $r(n,t) = \text{the minimum of } k_i(n,t) \text{ and } e(n,t)$
- if $M(n,t) > 0$ and $M(n,t) \geq k_i(n,t)\Delta t$,
then $r(n,t) = k_i(n,t)$ (3.2)
- if $M(n,t) > 0$ and $M(n,t) < k_i(n,t)\Delta t$,
then $r(n,t) = \text{the minimum of } k_i(n,t) \text{ and } \{e(n,t) + M(n,t)/\Delta t\}$

The first case represents a situation where no excess mass is exposed. Under these conditions, the release rate is controlled by whichever of the two rates is smaller. The second case represents a situation in which there is an excess of exposed (available) mass in the immediate vicinity of the waste package. In this case, the release rate is controlled only by the rate of mass transfer. The last case ensures that mass accounting errors are not incurred as a result of the discretization of time in the computational solution.

Others (e.g., Sadeghi et al., 1989) have typically considered three types of releases: 1) solubility-limited releases, 2) congruent releases from the waste matrix, and 3) releases of readily soluble species. After describing the calculation of $e(n,t)$ and $k_i(n,t)$ in detail in the following sections, the manner in which the above methodology accommodates each of these types of releases will be summarized.

Note that in the discussion above, $e(n,t)$, $k_i(n,t)$, $r(n,t)$, and $M(n,t)$ referred to a single waste package only. Hence, the calculations would need to be carried out for each individual waste package and summed over all waste packages to obtain the total repository release. In order to

accurately represent uncertainty and waste package-to-waste package variability, however, such an approach would be prohibitive in terms of computational expense (i.e., a large number of individual waste packages would need to be simulated every realization). To avoid this difficulty, RIP takes a different approach and *does not simulate individual waste packages*. Instead, RIP divides the population of waste packages in the repository into a discrete number of *waste package groups*. These groups are used to represent repository-wide random variability in near-field environmental conditions. How these groups are defined will be discussed in detail in Section 3.3. For the present purposes, however, it is sufficient to note that $e(n,t)$, $k_t(n,t)$, and $r(n,t)$ represent the mass exposure rate, mass transfer rate, and mass release rate *not for a single waste package, but for a group of waste packages*. Release from the entire repository is calculated by summing the contributions from each group. This simplification has important implications for the interpretation of $k_t(n,t)$ and the resulting release rate, and will be discussed again in subsequent sections.

Finally, it is important to remember that the release rate represents the total rate of release *from* the waste packages. It says nothing about where the radionuclides are released *to*. The RIP integrated model, however, as noted in Chapter 2, consists of components describing transport pathways, disruptive events and fate and effect, in addition to the waste package behavior component. The transport pathways component model defines the transport pathways along which radionuclides can migrate, linking the waste packages to the accessible environment. When the radionuclides are released *from* the waste packages (as defined by $r(n,t)$), they will be released *to* one or more transport pathways. The available pathways will be defined within the transport pathways component model. The user must specify how a particular nuclide released from a particular type of waste package is partitioned into the various transport pathways. This partitioning may, in some cases, be controlled by environmental conditions. Where the transport pathways are defined to begin is entirely up to the model user. For example, consider a waste package emplaced in a borehole with a backfilled annulus. The waste package model could be used to simulate mass transfer out of the container and through the annulus, with one or more transport pathways beginning at the edge of the borehole. Alternatively, the waste package model could simulate mass transfer out of the container, with one or more transport pathways beginning at the edge of the container, simulating mass transfer through the annulus and subsequently into the rock. These two conceptual approaches would be differentiated by the specification of mass transfer parameters, as discussed in Section 3.2.4. The transport pathways model is described in detail in Chapter 4.

Details of waste package failure rates and the subsequent radionuclide exposure and transfer rates are presented in the following sections.

3.2.2 Waste Package Failure Rates

The overall radionuclide exposure rate is a function of the rate at which the waste package containers are failing. RIP explicitly considers two layers of waste package containment: the *primary container* (the outside waste package itself), and the *secondary container* (e.g., the cladding for spent fuel or the pour canister for high level defense waste). Note that whenever the word "container" is used alone, the primary container is implied.

As discussed above, rather than explicitly modeling failure mechanisms in detail, waste package failure is represented in terms of high level phenomenological parameters: distributions of container lifetimes. Similar approaches have been used by others (e.g., Bullen, 1990). The manner in which these failure distributions are represented and computed is described below.

3.2.2.1 Primary Container Failure Rate

The general shape of a primary container failure distribution is shown in Figure 3-3. This is a density function of failure frequency. Failure is defined as the initial breaching of the container. In this figure, a waste package has only two states: unfailed or completely failed. The y-axis, $c(t)$, represents the fraction of containers failing at a given time, and the x-axis represents time of failure. This distribution can be thought of equivalently as a container failure rate plotted versus time after repository closure. The integral over time of $c(t)$ would produce the actual fraction of containers that had been breached by a given time.

The shape of $c(t)$ depends on the actual failure modes (such as uniform corrosion, pitting, etc.) that are of importance. The model assumes that it is possible to develop a separate failure distribution for each failure mode. The failure modes are then combined in an appropriate manner to obtain $c(t)$. Appendix E describes in detail the manner in which the separate failure modes are mathematically combined. It is assumed that the different modes operate independently and without synergism. For the purposes of illustration, Figure 3-3 represents the combination of three failure modes: one due to flawed packages or emplacement, and two that represent different corrosive mechanisms.

Mode 1 in the figure represents the failure of containers due to flawed packages and/or flawed emplacement. This process might be represented by an exponential distribution. Modes 2 and 3 represent the failure of containers due to two different corrosion mechanisms. A number of distributions could be used to describe these corrosive failure modes. One such distribution is the Weibull distribution, which is used in many engineering applications to predict component failure. As shown in Figure 3-3, the three distributions describing the different failure modes are combined to produce the total failure distribution $c(t)$.

Each of the independent failure mode distributions must be described by one or more parameters (e.g., the Weibull distribution requires three parameters). Two other pieces of information are also required to define a container failure mode distribution: 1) the probability that the mode is active at any given waste package (e.g., only a small fraction of the waste packages will be susceptible to failure due to flawed packages or emplacement); and 2) whether the mode can start immediately upon closure or cannot start until the waste package is rewet (after drying out due to the thermal pulse). The rewetting time is a function of the thermal and moisture conditions in the vicinity of the waste package and will be discussed in detail in Section 3.3.

The mathematical details of the most common distributions that are likely to be used to represent container and cladding failure (the exponential, Weibull, uniform, and degenerate) are discussed in Appendix F.

FIGURE 3-3
PRIMARY CONTAINER FAILURE DISTRIBUTION
ARGONNE/MODEL DEVELOPMENT

3.2.2.2 Secondary Container Failure Rate

Once a particular primary container fails, it is necessary to determine the distribution of failure times for the secondary container (for spent fuel, the cladding surrounding the rods within that container; or analogously for vitrified high-level waste, the distribution of failure times for the pour canister). The secondary container failure distribution for a primary container that has been breached at a given time is shown in Figure 3-4. Like the primary container failure distribution, this is a density function of failure frequency. Failure is defined as the initial breaching of the secondary container, and there are only two possible states: unfailed or completely failed. The y-axis, $w(t, \Theta)$, represents the fraction of failed secondary containers at a given time within a group of primary containers that fail at time Θ , and the x-axis represents time of secondary container failure. This distribution can be thought of equivalently as a secondary container failure rate plotted versus time after closure. The integral over time of $w(t, \Theta)$ would produce the actual fraction of secondary containers (whose primary container failed at time Θ) that had been breached by a given time t .

Like the primary container failure distribution, the shape of $w(t, \Theta)$ depends on the actual secondary container failure modes that are of importance. The model assumes that it is possible to develop a separate independent failure distribution for each failure mode. The failure modes are then combined in an appropriate manner to obtain $w(t, \Theta)$ (as detailed in Appendix E). It is assumed that the different modes operate independently (without synergism). For the purposes of illustration, Figure 3-4 represents the combination of three failure modes: one due to internal processes, and two that represent different corrosive mechanisms.

Mode 1 in Figure 3-4 represents failure due to internal processes. A spike exists at time = 0, representing the fraction of secondary containers (e.g., cladding) that has failed prior to repository closure due to other processes (transportation damage, internal processes, etc.). The tail of mode 1 represents the failure of the secondary container after closure but prior to actual primary container failure due to additional internal processes. This might be represented by an exponential distribution. Modes 2 and 3 represent the secondary container failure due to corrosion mechanisms following primary container failure. Like the primary container failure distribution, each of these mechanisms could be represented by a Weibull distribution.

In addition to the parameters describing the various independent failure modes, Θ , the time of actual primary container failure, is also required to fully define the shape of the total secondary container failure distribution. It is important to remember that Figure 3-4 is effectively the secondary container failure distribution for a group of primary containers that have been breached at a given time Θ . Hence, the actual shape of the distribution is directly related to the time of primary container failure, with a unique secondary container failure distribution associated with each primary container failure time. It is assumed in this model that the time of primary container failure does not affect the values of the other parameters describing the distribution. That is, the only difference between a secondary container failure distribution with primary container failure occurring at time Θ and a second distribution with primary container failure occurring at time $\Theta + \Delta t$ is that in the latter distribution, certain components of the total

Note: Secondary container is cladding for spent fuel; pour canister for HLDW.

FIGURE 3-4
SECONDARY CONTAINER FAILURE DISTRIBUTION
 ARGONNE/MODEL DEVELOPMENT

failure distribution (in this example, the Weibull portions of the distribution) are correspondingly shifted to the right (i.e., increasing time).

Two other pieces of information are needed to define a secondary container failure mode distribution: 1) the probability that the mode is active at any given waste package; and 2) whether the mode can start immediately upon closure or cannot start until the primary container fails.

3.2.2.3 Rate of Aging for Containers

The choice of using Weibull (or other distributions) to define the failure rates as a function of time is convenient but has a serious shortcoming. Because the parameters of the distributions defining primary and secondary container failure rates (e.g., the three parameters describing the Weibull distribution) cannot vary with time (i.e., a parameter that defines a distribution in time cannot vary with time), it is not possible for the failure rates to respond directly to changing environmental conditions. That is, the failure distribution for a given mode must be defined assuming a given set of conditions. Any temporal changes in environmental factors (e.g., temperature, saturation) that may affect the failure distribution must be known prior to its specification and indirectly incorporated into the form of the distribution:

Because such an approach limits the manner in which time-varying effects can be simulated, an additional feature is incorporated into the RIP model to increase flexibility. This feature allows the failure rates to respond directly to time-varying environmental factors. As described above, all failure mode distributions must be defined in terms of a standard set of constant environmental conditions. Each mode, m , however, has associated with it an additional parameter, known as the rate of aging, $R_{age}(m)$. The rate of aging can be a function of environmental conditions (which, as will be described in Section 3.3, may be temporally variable). For example, the aging rate could be specified to increase with increases in temperature or pH.

It is easiest to illustrate the use and physical significance of this parameter by considering an example. Suppose that $R_{age}(m)$ for a certain failure mode was described as a function of temperature such that at a certain elevated temperature the container aged (i.e., failed) at twice the rate as under the standard temperature under which the failure distribution for the mode was defined. If the container was subjected to this elevated temperature for, say the first 1000 years, the *effective age* of the container (with respect to that failure mode) would then be computed as 2000 years, twice the actual age. Hence, if the original failure distribution was defined such that 25% of the containers failed within 1000 years, and 60% of the containers failed within 2000 years, the model would compute that under the elevated temperature conditions, 60% of the containers would fail within 1000 years.

This approach has the effect of stretching and/or shrinking the time axis of the defined failure mode distributions. The effective age of the containers with respect to each mode is continuously tracked. For example, if a mode was not active under certain temperature conditions, $R_{age}(m)$ would be zero, and the effective age of the containers with respect to that

mode would not change with time. Note that if $R_{age}(m)$ is always equal to one, the effective age of a container is equal to the actual age.

Due to computational considerations, aging rates are only applied to primary container failure rate calculations and are not currently incorporated into secondary failure rate calculations. As a result, secondary container failure rates cannot respond directly to temporally changing environmental factors.

3.2.2.4 Discretization of Failures

The manner in which container failures are discretized is important to understand, as it effects how the user-defined failure distributions are actually represented by the computational model.

Referring back to Figure 3-3, integrating under the curve from 0 to some time t results in the fraction of the primary containers that have failed by time t . Multiplying this fraction by the total number of primary containers in the repository results in the number of containers that have failed by time t . In RIP, primary containers fail discretely. That is, it is not possible for a fractional number of containers to have failed at any given time. The implications of this are best illustrated by example, as shown in Figure 3-5.

Suppose that the primary containers were assigned a uniform failure distribution from 0 to 8000 years. For this example, we assume that there are only 5 primary containers. We first consider the case in which the computational time step is 100 years. Since RIP fails primary containers discretely, the first container fails when the cumulative failure distribution is equal to $1/5$ (time = 1600 years), the second container fails when the cumulative failure distribution is equal to $2/5$ (3200 years), and so on. In this case, the discrete failure times (e.g., 1600) are multiples of the time step.

If the time step is increased to 1000 years, the behavior is significantly different. The first container fails at the first multiple of the time step greater than or equal to 1600 (in this case, 2000), the second container fails at the first multiple of the time step greater than or equal to 3200 (4000), the third container fails at the first multiple of the time step greater than or equal to 4800 (5000), and so on.

Hence, the actual failure distribution simulated by the program depends on both the requirement that only integer numbers of containers can be failed, and on the degree to which the system is temporally discretized. Of course, for large numbers of waste packages, the importance of the first issue is less important. Recall, however, that failure distributions are computed for each waste package group, so that even though the total number of waste packages may be large, the number in a particular group could be quite small. It is critical for the user to be aware of these issues when defining failure distributions.

In the current version of RIP, secondary container failure *is not discretized*. That is, it is possible for a fractional number of secondary containers to have failed at any given time.

FIGURE 3-5
**DESCRETIZATION OF PRIMARY
 CONTAINER FAILURE**
 ARGONNE/MODEL DEVELOPMENT

3.2.3 Mass Exposure Rates

As described in Section 3.2.1, the radionuclide release rate for radionuclide n at time t , $r(n,t)$, is a function of the rate at which mass is exposed, $e(n,t)$, the maximum rate of mass transfer out and away from the waste package, $k_t(n,t)$, and the total amount of available (previously exposed) mass, $M(n,t)$. The manner in which the exposure rates are computed is described below.

Mass exposure is brought about by failure of the primary and secondary containers and exposure of the radionuclide mass to the surrounding environment. In other words, *exposed* implies that the mass is *made available* for mass transfer away from the waste package. Nevertheless, exposure does not imply that mass transfer can immediately take place. Mass transfer itself requires certain conditions. For example, if a waste package fails under dry conditions, although the mass is exposed, a non-gaseous radionuclide cannot be transferred in the absence of water. As will be seen in the next section, this dependence is built directly into the mass transfer rates.

The model assumes that the exposure rate for a given radionuclide is made up of three additive components:

- A portion of the inventory is located between the secondary container (e.g., cladding) and the primary container wall and is assumed to be exposed instantaneously upon primary container failure. This is referred to as the "free" inventory.
- A portion of the inventory is located in the gap between the secondary container (e.g., cladding) and the waste matrix, and is assumed to be exposed instantaneously upon secondary container failure. This is referred to as the "gap" inventory. For spent fuel, some species in this inventory will tend to be present at grain boundaries and exposed surfaces of the fuel. It is assumed that these species are exposed instantaneously along with the gap inventory upon cladding failure.
- The remaining portion of the inventory is bound within the waste matrix and is assumed to be exposed only upon alteration and/or dissolution of the matrix itself. This is referred to as the "bound" inventory.

Note that these three categories, although slightly different, are similar to those considered by others (e.g., Johnson et al., 1985; O'Connell and Drach, 1986; Apted et al., 1987).

Since each of these three inventories is exposed in a different manner, it is necessary to compute the exposure rate for radionuclide n at time t for each of the three inventories and sum these values to obtain the total exposure rate:

$$e(n,t) = e_f(n,t) + e_g(n,t) + e_b(n,t) \quad (3.3)$$

where:

- $e(n,t)$ = the total exposure rate for radionuclide n at time t [M/t];
- $e_f(n,t)$ = the exposure rate for radionuclide n in the free inventory at time t [M/t];
- $e_g(n,t)$ = the exposure rate for radionuclide n in the gap inventory at time t [M/t];
and
- $e_b(n,t)$ = the exposure rate for radionuclide n in the bound inventory at time t [M/t].

These three components can be computed as functions of the following parameters:

- $c(t)$ = primary container failure rate at time t [1/t];
- $w(t,\Theta)$ = secondary container failure rate at time t for a primary container that has failed at time Θ [1/t]
- $I_f(n,t)$ = free inventory of radionuclide n *per unfailed container* at time t (e.g., that portion located between the cladding and the container wall) [M];
- $I_g(n,t)$ = gap inventory of radionuclide n *per unfailed container* at time t (e.g., that portion located in the gap between the fuel and the cladding) [M];
- $I_b(n,t)$ = bound inventory of radionuclide n *per unfailed container* at time t (e.g., that portion bound in matrix) [M];
- $k_{a/d}(t)$ = fractional alteration/dissolution rate of waste matrix [1/t]; and
- N_c = number of containers.

$c(t)$ and $w(t,\Theta)$ have been discussed in Section 3.2.2. $I_f(n,t)$, $I_g(n,t)$, and $I_b(n,t)$ define the radionuclide inventory in an unfailed container. These inventories change with time due to decay processes (some nuclides decreasing and others increasing due to the production of daughter products). $k_{a/d}(t)$ is the alteration/dissolution rate of the waste matrix. $k_{a/d}(t)$ can be a function of environmental parameters (e.g., temperature and moisture), as will be discussed in Section 3.3.

Recall that the mass exposure rate, $e(n,t)$, is computed for each waste package group.

3.2.3.1 Free Exposure Rate

The exposure rate for that portion of the waste that is exposed instantaneously upon primary container failure is directly proportional to the container failure rate distribution:

$$e_f(n,t) = N_c \times (\text{free inventory}) \times (\text{container failure rate}) \quad (3.4)$$

$$e_f(n,t) = N_c \times I_f(n,t) \times c(t)$$

3.2.3.2 Gap Exposure Rate

The exposure rate for that portion of the waste that is exposed instantaneously upon secondary container failure is somewhat more complex:

$$e_g(n,t) = N_c \times (\text{gap inventory}) \times (\text{rate at which matrix becomes unprotected}) \quad (3.5)$$

$$e_g(n,t) = N_c \times I_g(n,t) \times g(t)$$

The matrix becomes "unprotected" when both the primary and the secondary container have failed. Hence, the rate at which matrix becomes unprotected, $g(t)$, is a function of both the primary and secondary container failure rates:

$$g(t) = \int_0^t [c(t) \times w(\tau, t) + c(\tau) \times w(t, \tau)] d\tau \quad (3.6)$$

The first term in the integral represents the contribution from those primary containers that are instantaneously failing at time t whose secondary container had previously failed due to internal processes. The second term represents the contribution from primary containers that had failed prior to time t whose secondary container is instantaneously failing at time t .

3.2.3.3 Bound Exposure Rate

The exposure rate for that portion of the waste that is exposed upon alteration/dissolution of the matrix is a function of the mass of radionuclide that is unprotected (i.e., primary and secondary container have failed) but is still bound in an unaltered/undissolved matrix, and the alteration/dissolution rate of the matrix:

$$e_b(n,t) = N_c \times (\text{fraction of mass that is unprotected, but unaltered/undissolved}) \times (\text{matrix alteration/dissolution rate}) \times (\text{bound inventory}) \quad (3.7)$$

$$e_b(n,t) = N_c \times M_{uu}(t) \times k_{a/d}(t) \times I_b(n,t)$$

Note that this equation assumes that *exposure* of bound nuclides is controlled by dissolution/alteration of the matrix. (As will be seen in the following section, however, *release* of bound nuclides may be controlled by individual radionuclide solubility considerations.)

$M_{uu}(t)$, the fraction of unprotected, unaltered, undissolved matrix, can be determined by solving the following differential equation:

$$dM_{uu}(t)/dt = (\text{rate at which matrix is being unprotected}) - (\text{rate at which unprotected matrix is being altered/dissolved})$$

$$dM_{uu}(t)/dt = g(t) - M_{uu}(t) \times k_{a/d}(t) \quad (3.8)$$

Since $k_{a/d}$ may be described as a function of time and $g(t)$ is complex, Equation 3.8 cannot be solved analytically and is solved numerically using a first-order finite difference approximation:

$$M_{\text{un}}(t) = \frac{M_{\text{un}}(t - \Delta t) + g(t) \Delta t}{1 + k_{a/d}(t) \Delta t} \quad (3.9)$$

To improve the accuracy of the finite difference approximation, Equation 3.9 is solved by subdividing the original computational time step.

Note that $k_{a/d}$ in Equation 3.9 represents any process that can act to expose nuclides that are bound in the matrix. It is assumed that this can come about by two types of processes: 1) aqueous alteration/dissolution of the matrix; and 2) air alteration of the matrix. Air alteration is included because it may greatly increase the surface area of the matrix, effectively exposing bound nuclides. Hence, $k_{a/d}$ is computed as a sum:

$$k_{a/d} = k_{\text{wat}} + k_{\text{air}} \quad (3.10)$$

where:

k_{wat} = aqueous alteration/dissolution rate of matrix [1/t]; and

k_{air} = air alteration rate of matrix [1/t].

Note that both k_{wat} and k_{air} may be described as functions of environmental conditions, and, as a result, it is likely that they will not occur simultaneously (e.g., k_{air} may only occur at high temperatures before the waste package rewets).

The air alteration rate, k_{air} , is directly specified by the user.

k_{wat} is specified in the model as follows:

$$k_{\text{wat}} = R_{\text{dis}} \times S \times f_w \quad (3.11)$$

where:

R_{dis} = matrix alteration/dissolution rate [$M/L^2/t$];

S = effective surface area of waste matrix in a failed container per unit mass [L^2/M]; and

f_w = fraction of waste matrix surface area in a failed container that is wet.

k_{wat} is automatically set to zero under dry conditions (i.e., at temperatures above the rewetting temperature, discussed below in Section 3.3.4). Note that R_{dis} , the aqueous matrix alteration/dissolution rate, can be described by the user as a function of local environmental conditions (e.g., temperature, chemistry). In some cases, the user may also wish to couple it to parameters describing mass transfer processes (discussed in Section 3.2.4).

The fraction of the waste matrix surface area that is wet, f_w , can also be described by the user as a function of environmental conditions. In addition, the user has the option of describing f_w as a function of the *mode of primary container failure*. This allows one to take into account the fact that the size and nature of container perforations vary depending on the failure mode, and as a result, the nature and characteristics of water contact with the waste matrix can be affected.

As described in detail in RIP User's Guide, if the user chooses to describe f_w as a function of failure mode, he/she must enter the fraction of waste matrix surface area that is wetted, $f_{w,m}$, for each primary container failure mode m . These are then combined to form the value of f_w used in Equation 3.11 as follows:

$$f_w = \frac{\sum_{m=1}^{NM} N_m \times f_{w,m}}{N_T} \quad (3.12)$$

where:

$$N_m = N_c \int_0^t c_m(\tau) d\tau \quad (3.13)$$

$$N_T = N_c \int_0^t c(\tau) d\tau \quad (3.14)$$

and

- N_m = cumulative number of containers that have failed by mode m ;
- N_T = cumulative number of containers that have failed by any mode;
- N_c = total number of containers;
- NM = total number of container failure modes;
- $c(t)$ = total container failure rate at time t [1/t]; and
- $c_m(t)$ = container failure rate by mode m at time t [1/t].

Note that for containers that fail due to disruptive events, the value of $f_{w,m}$ used is the highest of the values specified for the regular failure modes.

By definition,

$$\sum_{m=1}^{NM} N_m \geq N_T \quad (3.15)$$

As a result, Equation 3.12 implies that the effects of failure modes are additive. That is, if a container fails by two modes, one of which wets 10% of the surface, and another that wets 5% of the surface, the model assumes that 15% of the surface is wetted. In reality, the failures may not be independent (i.e., the failures may affect the same part of the waste package). Therefore assuming that the failures are additive is somewhat conservative. Note the that model automatically ensures that f_w is less than or equal to one.

As pointed out above, use of failure modes to describe f_w is entirely optional. That is, a single value of f_w , independent of failure mode, may be used directly in Equation 3.11 if desired.

The radionuclide exposure rate distributions with time are illustrated schematically in Figure 3-6.

3.2.4 Mass Transfer Rate

Even after a given mass of radionuclide is exposed, it is not considered to be released until the mass is physically transferred away from the immediate vicinity of the waste package. This transfer occurs via advective and/or diffusive processes, and is described by a parameter defining the maximum possible rate of mass transfer for a given radionuclide, $k_i(n,t)$.

It is important to differentiate the mass transfer rate out of the waste package from the mass transfer rate through transport pathways (discussed in Chapter 4), and to describe how these are related. The RIP waste package component model computes a maximum possible mass transfer rate *out of the waste packages*. As discussed previously, this is equivalent to the maximum possible mass transfer rate into the beginning of a transport *pathway*. Theoretically, if transport through the pathway is rapid, it will have no effect on the mass transfer rate out of the waste package (i.e., mass is diffused or advected away as soon as it is released into the pathway). If a "bottleneck" exists at the beginning of the pathway, however, this would influence the mass transfer rate out of the waste package (essentially causing exposed mass to accumulate at the waste package). In the current RIP algorithm, however, this is not accounted for within the waste package model and *mass transfer out of the waste package is independent of mass transfer through the pathway to which the mass is released*.

Instead, this is accounted for within the transport pathways component model.

Algorithmically, a bottleneck in the first pathway will act to accumulate mass in the beginning of the pathway. As a result, simulated waste package releases may be overestimated if pathway bottlenecks are present. Nevertheless, accumulating mass at the beginning of the first pathway (as opposed to at the waste package itself) produces similar results in terms of mass transport *through the entire system*.

As pointed out in section 3.2.1, $e(n,t)$ and $k_i(n,t)$ represent the mass exposure rates and the mass transfer rate, not for an individual waste package, but for a group of waste packages. Hence, $k_i(n,t)$ represents the total amount of mass that can be transferred from a defined group of waste packages. It is computed as the product of the mass transfer rate from a single failed container, $k_{ip}(n)$, and the total number of *primary* failed containers in that group.

FIGURE 3-6
RADIONUCLIDE EXPOSURE DISTRIBUTION
ARGONNE/MODEL DEVELOPMENT

As will be discussed in Section 3.3, such an approach allows the user to more easily represent waste package-to-waste package variability in near-field conditions throughout the repository. However, this approach also imposes some limitations on the manner in which mass transfer away from the waste package can be represented, and the user must have an understanding of these limitations.

First, this approach implicitly assumes that all of the exposed mass at individual waste packages is evenly distributed between the failed packages within a given group. In reality, the exposed mass may be concentrated in a fraction of the failed containers (e.g., those that have failed recently). Assuming that the exposed mass is evenly distributed throughout the group results in an overestimate for $k_i(n,t)$. This is because mass transfer from a single waste package can be limited by solubility considerations and/or limited water flux. Spreading the same mass over a group of waste packages reduces both of these limitations, increasing the maximum possible mass transfer rate. This limitation can result in conservative (overestimated) mass transfer rates.

The second limitation is that mass transfer rates can not be described as a function of the time of container failure. This is because the mass transfer rate is represented by a single value for a particular group, although individual waste packages within a group do not necessarily fail at the same time. As a result, only a *steady-state* mass transfer rate can be used. Because it represents the mass transfer rate for the entire group, it must be independent of the time at which the container was breached and mass transfer away from the package commenced. In effect, transient solutions for mass transfer from individual waste packages can not be directly represented by the waste package component model.

Nevertheless, in situations where it is important to represent such transient effects (e.g. diffusion through a sorptive buffer), RIP allows the model user to do so by defining transport pathways appropriately (within the transport pathways component model). As discussed in Section 3.2.1, the user is free to define exactly where the waste package model ends and the transport pathways model begins. For example, if diffusion of radionuclides through a rubble-filled annulus was important to consider, the user could define an "annulus" pathway (or pathways) beginning at the edge of the container. Since the transport pathways component model explicitly simulates transient mass transfer (including the effects of retardation), the transient behavior within the backfill could be represented. Representing transient waste package release is discussed in more detail in Section 3.2.4.3.

The computation of k_{tp} for both aqueous and gaseous species, is detailed below.

3.2.4.1 Mass Transfer of Aqueous Radionuclides

Advective Mass Transfer

For an aqueous radionuclide, n , the maximum possible mass transfer rate from a single waste package, is computed as a sum of advectively-controlled mechanisms and diffusively-controlled mechanisms:

$$k_{tp}(n) = k_{tp,a}(n) + k_{tp,d}(n) \quad (3.16)$$

where:

$k_{tp,a}(n)$ = maximum possible advective mass transfer rate for radionuclide n [M/t];
and

$k_{tp,d}(n)$ = maximum possible diffusive mass transfer rate for radionuclide n [M/t].

Note that both $k_{tp,a}(n)$ and $k_{tp,d}(n)$ are automatically set to zero prior to rewetting of the waste package.

The maximum possible *advective* mass transfer rate is computed as follows:

$$k_{tp,a}(n) = \text{FLOW} \times \text{CATCH} \times C(n) \quad (3.17)$$

where:

FLOW = repository level groundwater flow rate [L/t];

CATCH = effective cross-sectional catchment area (perpendicular to the flow) associated with a single waste package; it is multiplied by the repository level flow rate to compute the effective volume rate of flow of water that is at a concentration of $C(n)$ [L²];

$C(n)$ = concentration of radionuclide n in water at the waste package [M/L³].

Note that FLOW $\times$ CATCH essentially quantifies the effective volume of water that reaches the concentration $C(n)$. Hence, for purely advective transport (e.g., such as the situation illustrated in the left side of Figure 3-1), the mass transfer rate is assumed to be proportional to the volume rate of flow of water coming into contact with the waste. It is further assumed that this water is at a given effective concentration that, as will be detailed below, is either controlled by the solubility of the constituent or by the radionuclide's inventory. FLOW and CATCH are directly specified by the user. $C(n)$ is computed internally as will be specified below.

Diffusive Mass Transfer

The maximum possible *diffusive* mass transfer rate is computed as follows:

$$k_{tp,d}(n) = D_{\text{eff}}(n) \times \omega \times C(n) \quad (3.18)$$

where:

$D_{\text{eff}}(n)$ = the effective diffusion coefficient for radionuclide n (taking into account tortuosity) [L²/t];

ω = geometric factor for diffusive mass transfer [L]; and

$C(n)$ = concentration of radionuclide n in water at the waste package [M/L³].

Note that this formulation implicitly assumes a zero concentration boundary condition (since only one concentration term, that of the source, is included in Equation 3.18).

$D_{eff}(n)$ and ω are directly specified by the user. A large number of formulations are available in the literature for describing diffusive mass transfer (e.g., Kerrisk, 1984; Aidun et al., 1988; Sadeghi et al., 1989; Pigford et al., 1990). Recall that only steady-state formulations can be used in the RIP model. As discussed previously, the form of $D_{eff}(n)$ and ω will depend on how the subsequent transport pathways into which the waste packages release mass are defined. As illustrative examples, two simple steady state formulations for ω are presented below.

Steady state diffusion from a bare spherical waste form of radius R through a medium with effective porosity η_e (Chambre et al., 1985):

$$\omega = 4\pi R \eta_e \quad (3.19)$$

Steady state diffusion through circular perforations in container wall (Aidun et al., 1988):

$$\omega = \frac{N_p \pi \eta_e a^2}{\left[\pi \frac{a^2}{4} + D_{eff,h} \eta_{e,h} L \right]} \quad (3.20)$$

where:

- a = radius of circular perforations [L];
- N_p = number of perforations;
- $D_{eff,h}$ = effective diffusion coefficient in perforation [L^2/t];
- L = thickness of container wall [L];
- η_e = effective porosity in backfill; and
- $\eta_{e,h}$ = effective porosity in perforation.

Note that these are just examples, and no specific formulation for ω is hard-coded into the program; the user must specify ω explicitly, and is free to use any form desired.

Computing the Effective Concentration

Both $k_{tp,a}(n)$ and $k_{tp,d}(n)$ require a value for $C(n)$, the effective concentration of the radionuclide in the water in contact with the matrix. This is calculated as follows:

$$C(n) = \text{MIN} \left[\frac{M_p(n)}{V_w + V_s(n)}, C_s(n) \right] \quad (3.21)$$

where:

$$M_p(n) = \frac{M(n, t)}{N_T} \quad (3.22)$$

and

- $M(n, t)$ = total exposed mass of radionuclide n at time t [M];
- N_T = cumulative number of primary containers that have failed by any mode (by time t);
- $M_p(n)$ = average exposed mass of radionuclide n per failed waste package [M];
- V_w = water volume in contact with matrix in failed waste package [L^3];
- $V_s(n)$ = equivalent volume due to sorption in waste package [L^3]; and
- $C_s(n)$ = saturation concentration of radionuclide n [M/L^3].

The term $V_s(n)$ accounts for the fact that not all of the radionuclide mass in a waste package will necessarily be dissolved. Some of it may be sorbed onto solids within the waste package. Assuming equilibrium partitioning, the mass sorbed within the waste package is equal to the product of $K_d(n)$, $C(n)$, and M_s , where $C(n)$ is as described above,

- $K_d(n)$ = the ratio of the mass sorbed per unit mass of solid to the dissolved concentration [$(M/M)/(M/L^3)$]; and

- M_s = the mass of sorbent (solid phase) in the waste package [M].

Given such a representation, $V_s(n)$ is defined as follows:

$$V_s(n) = K_d(n) M_s \quad (3.23)$$

K_d (which is nuclide specific) and M_s are directly specified by the user.

$C_s(n)$ is computed by the model as a function of the elemental solubility and the isotopic mass fraction of the entire waste package inventory. The user should be aware, however, that RIP only considers those isotopes that are specifically identified by the user. Isotopes that are not explicitly identified in the input data set (e.g., non-radioactive isotopes neglected by the user) are not considered in this calculation. Not including a significant isotope can result in computed saturation concentrations for other isotopes of the same element that are overestimated.

The formulation for $C(n)$ in Equation 3.21 is an attempt to account for highly soluble species whose effective concentrations may not be controlled by solubility considerations (i.e., the solubility is high and the concentration is determined by how much mass has been exposed and the volume of water into which it has dissolved). Note, however, that V_w may be a difficult

parameter to estimate. Specification of very small values for V_w and $V_s(n)$ is conservative in that it ensures that $C(n) = C_s(n)$.

Additional Comments on Aqueous Mass Transfer

Note that $k_{tp,a}(n)$ and $k_{tp,d}(n)$ can be described as functions of environmental conditions such that one of the two mechanisms will dominate under a given set of conditions. For example, in an unsaturated repository, under the "wet-drip" water contact mode, mass transfer is likely to be predominantly an advective process, while under the "moist-continuous" water contact mode, mass transfer may be predominantly a diffusive process (Apted et al., 1991). Note that if advection and diffusion are of similar importance, it may not be mathematically appropriate to add these two contributions independently. A more appropriate representation may be to specify ω such that one equation ($k_{tp,d}$) represents both advection and diffusion (e.g., Sadeghi et al., 1989), $k_{tp,a}$ being set to zero.

As discussed in the beginning of this section, k_{tp} represents the mass transfer rate from a single waste package. The model, however, does not simulate waste packages individually, but carries out calculations in terms of groups of waste packages. That is, k_t in Equation 3.2 is the mass transfer rate for a group of waste packages. Therefore, k_t is calculated as the product of the mass transfer rate from a single waste package and the total number of failed waste packages in the group:

$$k_t(n,t) = k_{tp}(n) \times N_T \quad (3.24)$$

As will be discussed in detail in Section 3.3, all of the parameters that define k_{tp} can be described in terms of environmental conditions. In addition, two of these parameters, FLOW and ω , can also be described as functions of the *mode of primary container failure* (completely analogous to f_w described in Section 3.2.3.3). This allows one to take into account the fact that the size and nature of container perforations vary depending on the failure mode, and as a result, the nature and characteristics of mass transfer can be affected.

If the user chooses to describe these parameters as functions of failure mode, a different value of the mass transfer coefficient results for each failure mode. That is, k_{tp} becomes subscripted by m ($k_{tp,m}$), where m is a subscript denoting failure mode. Rather than using Equation 3.24, $k_t(n,t)$ is then computed as follows:

$$k_t(n,t) = \sum_{m=1}^{NM} k_{tp,m}(n) \times N_m \quad (3.25)$$

Note that for containers that fail due to disruptive events, the value of $k_{tp,m}$ used is the highest of the values specified for the regular failure modes.

This equation is completely analogous to the calculation of f_w in Equation 3.12. That is, it essentially assumes that the effects of failure modes are additive. Hence, if a container fails by two modes, one of which produces a mass transfer rate of X , and another that produces a mass transfer rate of Y , the model assumes that the effective mass transfer rate for such a package is $X + Y$. In reality, the failures may not be independent (i.e., the failures may affect the same area

of the waste package). Therefore assuming that the failures are additive is somewhat conservative. However, if most waste packages fail by a mode that produces only restricted mass transfer, the model will be able to more realistically simulate the effects.

As was the case for the parameter f_w discussed in Section 3.2.3.3, use of failure modes to describe FLOW and ω is entirely optional. That is, single values for these parameters, independent of failure mode, may be used directly in Equations 3.17 and 3.18 if desired. To ensure consistency, however, the RIP user interface requires that if f_w is specified as a function of failure mode, FLOW and ω must also be specified as a function of failure mode. That is, either *all three parameters* (f_w , FLOW, and ω) are dependent on failure mode, or *all three* are independent of failure mode.

3.2.4.2 Mass Transfer of Gaseous Radionuclides

For gaseous radionuclides (e.g., ^{14}C), it is not appropriate to compute $k_{tp}(n)$ as a function of solubilities and fluxes. It is quite likely that mass transfer of gaseous radionuclides under unsaturated conditions will be relatively rapid (i.e., k_{tp} will be large). Under these conditions, the rate of exposure would always determine the release rate. However, because it is conceivable that physical situations may arise that limit the rate of gaseous mass transfer (e.g., localized saturation conditions, failed containers whose openings are "clogged"), the model allows the user to directly specify a mass transfer rate for gaseous constituents, $k_{tp,g}(n)$. Note that if gaseous mass transfer is rapid, $k_{tp,g}(n)$ is simply specified as a large number.

3.2.4.3 Representing Transient Mass Transfer

As mentioned previously, transient solutions for mass transfer from the waste packages can not be directly represented by the waste package component model. In situations where it is important to represent such transient effects (e.g. diffusion through a sorptive buffer), however, RIP allows the model user to do so by defining transport pathways appropriately (within the transport pathways component model). The transport pathways component model explicitly simulates transient mass transfer (including the effects of retardation).

The transport pathways component model is discussed in detail in Chapter 4. For the purposes of this discussion, suffice it to say that a particular transport velocity and dispersivity can be assigned to a pathway. The user could therefore represent transient mass transfer from a waste package by defining a "delay pathway" into which steady state releases from the waste package are directed. The velocity of the delay pathway would be described as a function of the parameters controlling diffusive mass transfer. For example, if we were attempting to represent transient diffusive mass transfer through a bentonite buffer, the transport velocity through the "delay pathway" would be defined as a function of the diffusivity and retardation factor for the radionuclide. While explicitly including these major controlling parameters (e.g., diffusivity, retardation), the function describing velocity could also be defined with a fitting parameter in such a way that the solution could be compared to and adjusted in order to better approximate appropriate analytical solutions to the diffusion equation.

Having defined a delay pathway with an appropriate velocity, the simplest way to represent the transient diffusive effect is to define the diffusive mass transfer rate as follows:

- 1) Prior to a delay time (defined as the ratio of the effective diffusive length to the diffusive velocity), the mass transfer rate is equal to 0;
- 2) After the delay time, the mass transfer rate is equal to the steady state value (computed by the waste package component model).

This results in a step function representation, as illustrated in Figure 3-7. This representation could be improved by assigning a dispersivity to the delay pathway (which could be adjusted based on comparisons with actual analytical solutions). This is also illustrated in Figure 3-7.

3.2.5 Summary of Radionuclide Release Calculation

As described in Section 3.2.1 and summarized in Figure 3-2, the release rate for a given radionuclide at a given time, $r(n,t)$, is computed as a function of the rate of exposure, $e(n,t)$, the maximum rate of mass transfer, $k_t(n,t)$, and the amount of previously exposed (but unreleased) mass at the waste package, $M(n,t)$. Recall that $M(n,t)$ is a function of the time histories of $e(n,t)$ and $k_t(n,t)$. The manner in which $e(n,t)$ and $k_t(n,t)$ are computed by RIP has been outlined in the previous sections.

As pointed out previously, others (e.g., Sadeghi et al., 1989) have typically considered three types of releases: 1) solubility-limited releases, 2) congruent releases from the waste matrix, and 3) releases of readily soluble species. Given the information presented in the previous sections, it is instructive to summarize how the methodology described above accommodates these three releases. The category that a particular radionuclide falls into is dependent on the specified input parameters.

Solubility-limited species, by definition, are controlled by the mass transfer rate, $k_t(n,t)$, which is dependent on solubility considerations (Equations 3.17 and 3.18). That is, for solubility-limited species, the exposure rate is faster than the rate at which mass can be transferred away (i.e., $e(n,t) > k_t(n,t)$), and the release rate is therefore equal to the rate of solubility-limited mass transfer (i.e., $r(n,t) = k_t(n,t)$). Note, however, that a species does not have to be solubility limited in order to be controlled by the mass transfer rate (i.e., the saturation concentration is just one parameter that affects the value of $k_t(n,t)$).

Similarly, for species that are controlled by alteration/dissolution of the waste matrix (congruent release), the exposure rate becomes the rate limiting step. That is, the release rate is equal to the exposure rate (i.e., $r(n,t) = e(n,t)$).

FIGURE **3-7**
**TRANSIENT DIFFUSIVE MASS
TRANSFER FROM WASTE PACKAGE**
ARGONNE/MODEL DEVELOPMENT

For readily soluble species (e.g., released from the fuel-cladding gap and grain boundaries), it can not be stated a priori whether exposure or mass transfer will control release. The important point to note is that the mass transfer rate is not calculated based on solubility considerations (which could be overly conservative since these species may be present at concentrations that are below solubility limits), but based on an estimate of the actual concentration at the waste package (Equation 3.21).

3.2.6 Simulating Different Waste Package Types

The previous sections have often referred to waste packages in terms of spent fuel waste. The methodology outlined above, however, is applicable to practically any kind of waste package. Obviously, the radionuclide inventories, alteration/dissolution rates, and failure distributions will differ for different waste types or designs. However, the computational structure and user-interface flexibility is such that RIP can accommodate almost any type of waste package that the user wishes to define.

The most important limitation of the methodology is that it is currently limited to explicitly considering no more than two layers of containment.

If more than one type of waste package needs to be considered within a simulation, it is necessary to specify a separate set of input parameters for each waste package type (e.g., one set pertaining to spent fuel waste packages, and one set pertaining to defense waste packages). That is, a number of the parameters previously introduced become subscripted by waste package type (e.g., $k_{air}(i)$, where i is waste package type). As described in the RIP User's Guide, the model can accommodate any number of different waste package types.

3.2.7 Incorporation of Disruptive Events

Disruptive events (such as earthquakes, volcanic activity, and human intrusion) may also affect the behavior of the waste package. Disruptive events are simulated in a separate RIP model component. The user defines the types of disruptive events that are possible, their probabilities of occurrence, and their consequences. The manner in which disruptive events are realized and simulated is discussed in detail in Chapter 5. Suffice it to say that their consequences will manifest themselves in the waste package model in three ways:

- A portion of the waste packages can be disrupted in place (e.g., due to mechanical failure induced by some disruptive event).
- A portion of the waste packages (and their inventory) can be moved directly to the accessible environment (AE) or some other location (e.g., the saturated zone).
- The parameters describing waste package behavior and/or environmental conditions for all or a portion of the waste packages may be changed (e.g., flooding of the repository, enhanced corrosion rates).

Note that disruptive events may also have other consequences that affect transport pathways to the accessible environment but do not directly affect the waste packages themselves (and are therefore not discussed here).

The first consequence, in which some portion of the waste packages are disrupted in place, is incorporated into the waste package model by automatically adding an additional primary container failure mode to the failure distributions. Such a failure mode is represented by a spike (mathematically represented by a Dirac delta function) at the time the event occurs. It is assumed that the secondary container instantaneously fails with the primary container. Hence, in addition to the container failure distribution, the cladding failure distribution $w(t, t_d)$ would also be affected (where t_d is the time of the disruptive event).

The second consequence listed above involves physically moving a portion of the waste packages with their inventory to the accessible environment or some other location (e.g., the saturated zone). In the model, this is represented by instantaneously releasing the corresponding radionuclide inventory to the specified location. It is assumed that the inventory released is equal to the inventory of the specified number of *unfailed* containers at the time of the event (i.e., even if the container failed prior to the event, it is conservatively assumed that most of the inventory would still be present within the waste package). It is also assumed that if the waste package is moved, all of its inventory is immediately released (the constituents are not limited by alteration or mass transfer processes).

The third consequence listed above is concerned with long-term effects on the repository system (e.g., raising the water table, opening a new transport pathway, changing the hydraulic gradient in the saturated zone). For example, one might specify an event that has a consequence of directly changing the value of mass transfer and/or corrosion parameters (perhaps as a result of a change in saturation or a temperature change).

Details of how disruptive event occurrences and consequences are specified are discussed in Chapter 5.

3.3 Representation of Near-Field Environmental Conditions

As pointed out in Section 3.2, the parameters controlling waste package behavior (i.e., the parameters describing the primary and secondary container failure distributions, exposure rates, and mass transfer rates) may be dependent on near-field environmental conditions. This section describes how near-field environmental conditions are represented and used in the waste package model.

Near-field environmental conditions are used by the waste package model in two ways:

- They are automatically incorporated into some of the algorithms that control waste package failure and radionuclide release described in the previous sections (e.g., the flow rate at repository level controls advective mass transfer, rewetting behavior can influence both failure rates and mass transfer rates).

- Parameters describing near-field environmental conditions (referred to here as *environmental factors*) can be used directly in the definition of any user-defined model parameter. That is, waste package model input parameters (e.g., matrix dissolution rate, radionuclide solubilities) can be defined by the user as direct functions of environmental factors (e.g., temperature, pH).

As described in Section 2.4, the RIP software is structured such that the user can define input parameters as functions of other user-defined parameters. What sets environmental factors apart from regular user-defined parameters is that they can be defined as having *variability* across the repository.

Recalling the discussion of uncertainty and variability in Section 3.2, it is possible for model parameters representing environmental factors to be both uncertain and variable. Variability should not be confused with uncertainty. Uncertainty in a model parameter implies a lack of knowledge regarding the actual value of the parameter. This is represented in RIP by describing the uncertain parameter as being stochastic (i.e., represented by a distribution). The parameter's distribution is sampled each realization. That single parameter value is then used throughout the realization. Variability in a model parameter, on the other hand, implies that for a given realization, a distribution of parameter values exist. That is, the parameter can vary from waste package to waste package in a given system realization. The mode of water contact at a waste package in an unsaturated repository is an example of a variable parameter (two different contact modes are schematically illustrated in Figure 3-1). Note that the variability that is represented here is a *random variability*. There are no spatial trends implied. The variability in a particular parameter occurs randomly throughout the repository.

Section 3.3.1 describes how variability of near-field environmental conditions is explicitly included in the model. Sections 3.3.2 and 3.3.3 discuss how two major variable environmental factors, temperature and moisture conditions, are represented in the model. As pointed out above, this does not imply that other factors (e.g., chemistry) must be excluded. Because moisture and temperature are clearly critical factors, however, they are explicitly "hard-wired" into the code and are discussed in detail below. The structure of the model is such that other variable environmental factors can easily be defined by the user if necessary, and this is discussed in Section 3.3.4. Finally, Section 3.3.5 describes how the drying and rewetting behavior of waste packages can be represented.

3.3.1 Representation of Variability Between Waste Packages

Waste package-to-waste package variability is incorporated in the model by internally discretizing the waste package population into a discrete number of *waste package groups*. Groups are defined as a function of both near-field conditions and waste package type (e.g., spent fuel, defense waste). That is, a particular waste package group includes waste packages of a particular type that are subject to a specific set of near-field conditions. As was discussed in Section 3.2.6, the user specifies the number of waste packages of each type that are emplaced in the repository. We describe here how waste package groups represent variable near-field conditions.

Near-field conditions are defined in terms of specified variable *environmental factors* (water contact mode, temperature, pH, redox conditions, stress, etc.). The user must determine which environmental factors he/she wishes to include in the model. Two environmental factors, water contact mode (i.e., moisture conditions) and temperature, are explicitly incorporated in the computational algorithm. As will be shown, the structure of RIP is such that other user-defined environmental factors can readily be added.

For each environmental factor that the user wishes to represent as being variable, it is necessary to define a distribution describing its variability. Based on additional user input (described in detail in the RIP User's Guide), RIP then converts the distribution describing the parameter's variability into an *equivalent discrete distribution*. (As will be discussed below, water contact mode is an exception to this rule: it's variability is directly specified in a discrete manner.)

As an example, consider a case in which we assume that the environmental conditions can be defined in terms of only two controlling variable environmental factors: the mode of water contact and the temperature. To further simplify the example, assume that the variability distributions of these controlling parameters are already discretized. Since the variability of these parameters is described in terms of discrete distributions, they will automatically define a discrete number of *waste package groups*. For example, if we define water contact mode in terms of three discrete categories (e.g., "wet-drip", "moist-continuous" and "dry"), and temperature conditions in terms of three discrete categories (e.g., "hot", "warm", "cool"), the waste package population would be divided into $3 \times 3 = 9$ waste package groups. If more than one waste package type is included in a simulation (e.g., spent fuel and defense waste), the population would also be distinguished by waste package type, resulting effectively in $3 \times 3 \times 2 = 18$ groups. This is illustrated schematically in Figure 3-8.

A certain fraction of the entire waste package population will be located in each of these groups. For example, if 30% of the waste packages are "wet-drip", 20% of the waste packages are "warm", and 80% of the waste packages are of the type "spent fuel", then the "wet-drip", "warm", "spent fuel" waste package group would contain $(0.3 \times 0.2 \times 0.8 = 0.048)$ 4.8% of the waste packages. (When computing the number of waste packages in each group, RIP rounds numbers to the nearest integer. Any deviation in the total number of waste packages is then corrected by adding or subtracting an appropriate number of waste packages to the largest group, while ensuring that the total number of packages of each type is preserved.)

Note that this representation of variability requires that the different environmental factors defined by the user be independent of each other (e.g., the distribution of water contact modes must be independent of the distribution of temperature).

Each environmental factor has a name by which it can be referenced (e.g., CONTAC, TEMP, pH). System parameters can be made dependent on environmental factors by referencing these names in a function (this is described in greater detail in the RIP User's Guide). The value of these parameters would therefore vary from group to group. Within the computational algorithm, at every time step within a realization RIP computes the release from each group, and then sums the results over all the groups to compute the total release from the repository. Note that although the parameters controlling waste package release are described in terms of

FIGURE **3-8**
**EXAMPLE OF DISCRETIZATION OF
 REPOSITORY INTO ENVIRONMENTAL GROUPS**
 ARGONNE/MODEL DEVELOPMENT

the entire group (e.g., exposure rate for the group, mass transfer rate for the group), it is important to understand that *the model does not assume that all waste packages within a group behave identically*. This is because within a group waste packages fail according to a defined failure distribution, with some waste packages failing earlier than others. As discussed in Section 3.2, this distribution of failure times is explicitly incorporated into the release calculation for a given group.

As discussed in Section 3.2, this method of incorporating variability results in some limitations, particularly regarding the representation of mass transfer. An alternative approach would involve simulating a large number of individual waste packages, the environmental conditions, failure times, and parameters describing mass exposure and mass transfer at each package being sampled from specified distributions. For each realization, however, a large number of individual waste packages would need to be simulated in order to adequately represent the full range of uncertainty in container failure times and the full range of variability in near-field environmental conditions. By simulating waste package groups (as opposed to individual waste packages) we are better able to represent the effect of this variability (since the failure rate distributions are explicitly included in the calculations analytically). Given the computational advantages of this approach, and the fact that the resulting limitations are not severe (see discussion in Section 3.2.4), the authors believe that the waste package group approach is appropriate.

The actual manner in which variable environmental factors are specified is presented in the following three sections.

3.3.2 Representation of Moisture Conditions - Water Contact Modes

The nature of the geological materials at actual repository sites is likely to be quite heterogeneous, producing a wide variety of moisture conditions and/or modes of water contact throughout the repository. As a result, treating all waste containers as if they will be subject to the same mode of water contact may be a very poor assumption. Various containers will be subject to different moisture conditions as a result of hydrogeological variability. This variability can be represented by a discrete distribution of water contact modes in the immediate vicinity of the waste packages. Figure 3-9 shows an example schematic of such a distribution. In this simple example, it consists of three categories: "wet drip", "moist-continuous" and "dry". These have been used to describe moisture conditions at an unsaturated repository such as Yucca Mountain (O'Connell and Drach, 1986; Apter et al., 1991). Note that the specification and definition of the various categories and the variability throughout the repository (i.e., what fraction of the containers are subjected to each mode) must be determined by the user.

The water contact mode is referenced by the user by assigning an integer value to the parameter CONTAC, each integer value indicating (i.e., acting as an identifier for) a different water contact mode. For each value of CONTAC (i.e., for each water contact mode) the user must specify the fraction of waste packages subjected to those conditions. Each waste package group would then have a particular value for CONTAC (in the example shown in Figure 3-6, "wet-drip", "moist-continuous", and "dry" refer to different values of CONTAC). Waste package

FIGURE 3-9
EXAMPLE OF WASTE PACKAGE
WATER CONTACT MODE DISTRIBUTION
ARGONNE/MODEL DEVELOPMENT

parameters may then be specified in terms of the water contact mode by referencing the parameter CONTAC. The specification and use of variable water contact modes, including the manner in which the distributions can be made to change in response to other environmental conditions (e.g., increased infiltration) is discussed in greater detail in the RIP User's Guide.

Note that the water contact mode variability is assumed to be due to local random hydrogeologic conditions at the scale of individual waste packages: it is not meant to represent large-scale spatial trends. In addition, note that the water contact mode represents the long-term distribution expected during the post-thermal period. That is, it is independent of the transient effect of heating in the vicinity of the waste package due to radioactive decay processes. Due to the thermal pulse, some waste packages may remain dry for long periods (and, if included in the contact mode distribution shown above, this would be manifested as a larger fraction in the "dry" category). Although this phenomenon can be represented in the model (as described below in Section 3.3.6), it is not represented by the water contact mode distribution, which only represents post-thermal conditions.

3.3.3 Temperature Conditions at Waste Packages

The second major variable environmental factor that influences waste package behavior is the temperature in the repository and at the waste packages. Temperature behavior is essentially a function of the inventory of the various waste packages, their age, the total number of waste packages, the repository design (e.g., spacing of the waste packages), and the thermal characteristics of the surrounding geologic materials. The moisture content of the repository will also affect thermal behavior (i.e., energy is used in heating and boiling water).

The temperature in the repository will change with time as the waste decays. The thermal behavior of the repository is represented in the RIP model by a parameter defined as the average temperature at the edge of a waste package as a function of time. This parameter is a function of waste package type:

$$\text{TEMPAV}_i(t) = T_m(t) + T_i(t) \quad (3.26)$$

where:

$\text{TEMPAV}_i(t)$ = the average temperature at the edge of waste package type i at time t ;

$T_m(t)$ = the mean effective temperature (in the rock) throughout the entire repository at time t ; and

$T_i(t)$ = the incremental temperature above the mean repository temperature at the edge of waste package type i at time t .

The user must directly specify the forms of $T_m(t)$ and $T_i(t)$. Figure 3-10 illustrates the anticipated form of $T_m(t)$ and $T_i(t)$. As described in the RIP User's Guide, the time histories $T_m(t)$ and $T_i(t)$ can be described stochastically to account for uncertainty.

Note: temperature at edge of waste package type 1 = $T_m + T_1$

FIGURE 3-10
 MEAN TEMPERATURE
 AS A FUNCTION OF TIME
 ARGONNE/MODEL DEVELOPMENT

Because some of the controlling parameters are likely to be variable (e.g., geologic materials in the repository are expected to be somewhat heterogeneous; waste packages will have different heat production rates depending on their type, their age, and where they are located within the repository), the actual temperature history at a waste package may vary significantly throughout the repository. This is represented in the model by defining the *variability* around the average temperature $TEMPAV_i(t)$ and creating a *discrete distribution* of temperature variability.

Specification of temperature variability is carried out in two steps. First the user specifies the form of a variability distribution that is used to modify the average temperature $TEMPAV$. We refer to the variability parameter as $TEMPV$. In the current version of RIP, the distribution of this parameter can be either triangular or uniform, and must be symmetric about the value 1 (e.g., a uniform distribution between 0.85 and 1.15). Having specified the distribution, the user then specifies how this distribution is to be discretized by defining several (up to six) cumulative probability levels (e.g., 0.33, 0.66, 1.0). RIP then discretizes the distribution by using the expected value of the ranges defined by the specified probability levels as the discrete values. For example, specifying a uniform distribution with a variability of 15% (0.85 to 1.15), and discretization at the 0.33, 0.66, and 1.0 cumulative levels, defines the following discrete distribution:

TEMPV	PROBABILITY
0.9	0.33
1.0	0.33
1.1	0.34

The distribution has been discretized into three discrete values corresponding to the three ranges defined by the specified probability levels: 0 to 0.33, 0.33 to 0.66, and 0.66 to 1.0. The discrete values for the distribution are computed as the expected value of each range (e.g., the 0.333 cumulative probability level corresponds to a value of 0.95; the expected value of a uniform distribution between 0.85 and 0.95 is 0.9). Note that if a triangular distribution had been specified, the values would have been different, since the expected value in each range will be shifted toward 1.0.

The three discrete values described above would define three temperature categories that define variability across the repository: 33% of the packages would have a temperature of $0.9 \times TEMPAV_i(t)$, 33% of the packages would have a temperature of $1.0 \times TEMPAV_i(t)$, and 34% of the packages would have a temperature of $1.1 \times TEMPAV_i(t)$. This is illustrated in Figure 3-11.

A single value of $TEMPV$ of 1.0 (implying no variability in temperature) is the default for RIP.

The actual temperature at a particular waste package is referenced by the internal environmental factor $TEMP$ (which is completely analogous to the environmental factor $CONTAC$ discussed previously). Other model parameters can subsequently be defined as a function of temperature, by referencing the name $TEMP$. At any given time, $TEMP$, as shown above, is computed internally by RIP as follows:

$$TEMP = TEMPV \times TEMPAV_i(t) \quad (3.27)$$

FIGURE 3-11
EXAMPLE OF TEMPERATURE DISTRIBUTION
AT WASTE PACKAGE EDGE
ARGONNE/MODEL DEVELOPMENT

In the example illustrated in Figure 3-8, "hot", "warm" and "cool" refer to different values of TEMPV (e.g., 1.1, 1.0, 0.9). Hence, in this simple example, TEMPV and CONTAC are the environmental factors that define the waste package groups. Since TEMPV varies between waste package groups, TEMP also varies between waste package groups.

3.3.4 Defining Other Variable Environmental Factors

As discussed above, although only two environmental factors are explicitly incorporated into RIP, the software is structured such that the user can define other environmental factors (e.g., pH, stress, redox conditions) whose variability the user wishes to include in the model. Hence, the user can add variability to nearly any waste package parameter he or she wishes to define.

The user first defines the name of the environmental factor (e.g., PH) and the average value about which the environmental factor's variability is to be centered (e.g., 7). Note that this average value need not be a constant, and may be described stochastically or as a function. A variability distribution is then defined in the same manner as described for temperature (e.g., 0.9, 1.0, 1.1). We refer to each of these discrete values in the distribution as the *variability factor* for each environmental factor category. In this example, we would refer to this factor as PH_V (that is, the environmental factor name with "_V" appended on to the end). PH_V is analogous to TEMPV discussed in Section 3.3.3. This would define a number of discrete PH categories (e.g., $0.9 \times 7 = 6.3$, $1.0 \times 7 = 7.0$, $1.1 \times 7 = 7.7$).

The user-defined environmental factor (in this case PH) is completely analogous to the environmental factors CONTAC and TEMP discussed previously. That is, other waste package model parameters could subsequently be defined as a function of the pH, which would be variable through the repository, by referencing the environmental factor name PH. In the example illustrated in Figure 3-6, adding the three pH categories (e.g., "acidic" corresponding to 6.3, "neutral" corresponding to 7.0, and "basic" corresponding to 7.7) would add a fourth dimension to the diagram, resulting in $3 \times 3 \times 2 \times 3 = 54$ waste package groups. As shown above, the actual value of the environmental factor (in this case, the pH) at any time in any particular group is computed as the product of the average value of the factor and the variability factor. In this example,

$$PH = (\text{average value of pH}) \times PH_V \quad (3.28)$$

Because PH_V varies from group to group, PH (which can be referenced by the user) varies from group to group.

The definition and use of environmental factors is discussed in more detail in the RIP User's Guide.

3.3.5 Rewetting Behavior for Waste Packages

For some repositories, after the waste is emplaced, radioactive decay of the waste can produce a thermal pulse that will evaporate water in the immediate vicinity of the packages. This pulse may be sufficient to keep the waste packages initially dry. As the waste packages subsequently cool (as the rate of radioactive decay decreases), the material in the vicinity of the waste packages will rewet. As discussed in Section 3.2, several waste package input parameters are sensitive to the rewetting behavior (e.g., container failure, matrix dissolution, and/or aqueous mass transfer may not proceed prior to rewetting).

Rewetting is a complex process dependent upon near field heat and moisture transport phenomena. Questions remain as to precisely how any given repository will behave thermally. Furthermore, the effect of the rewetting process can be quite complex. For example, even if the waste packages do dry out and rewet, mass transfer may be initially limited due to an inward advective gradient. Nevertheless, a simple rewetting model is given here. It is understood, however, that it may be necessary to expand on this simple model in the future to better simulate this complex process.

It is assumed here that a waste package is initially dry and remains dry for a time period t_{wet} , after which water is immediately allowed to contact the waste package (according to the moisture contact modes described above). In reality, this rewetting process will occur gradually, but for simplicity it is treated as an immediate process here (see Figure 3-12). The rewetting time, t_{wet} , is defined in terms of the temperature at which a waste package will become rewet, referred to here as T_r . Note that T_r may be described as a function of other environmental factors (e.g., water contact mode) if desired. Given a value for T_r , the temperature history for a given group of waste packages can then be used to directly determine at what time the waste package temperature reaches the rewetting temperature, thereby defining the rewetting time. This is illustrated graphically in Figure 3-13.

3.4 Model Input Parameters and Output Results

The type of input required by the RIP waste package model can be summarized into the following general categories:

- 1) *near field environmental conditions* (incorporating both waste package design features and environmental influences in the vicinity of the repository);
- 2) *waste package inventories, elemental properties* (e.g., solubilities), and *decay chains*;
- 3) *waste package (primary and secondary container) failure mechanisms*;
- 4) *mass exposure* (matrix dissolution and alteration) and *mass transfer parameters*; and
- 5) *disruptive events*:
 - a) definition and probabilities of disruptive event occurrences;
 - b) definition and probabilities of disruptive event consequences.

FIGURE 3-12
SCHEMATIC OF WASTE PACKAGE REWETTING
 ARGONNE/MODEL DEVELOPMENT

FIGURE 3-13
CALCULATION OF REWETTING TIME
ARGONNE/MODEL DEVELOPMENT

Note that the five general categories listed are not strictly independent of each other in that they are based on some of the same lower level information. For example, both when defining and generating the waste package failure mechanisms (item 3) or the near field environmental conditions (item 1), one must implicitly assume some specifics of waste package design and a general description of the range of potential environmental conditions. The reason that the required input parameters cannot be considered to be completely independent is that, for the most part, they are not low-level physically based parameters. As pointed out in Section 3.2, it is not practical at this time to build a model based on low-level physical parameters and first principles. Instead, the current model is based on subjective assessments of relatively high-level phenomenological parameters. In the list above, only items 2 and 5a could be considered to be low-level parameters. The rest can be considered high-level phenomenological parameters and must be based on expert interpretation of available data and more detailed modeling of processes. This is illustrated graphically in Figure 3-14. An ideal waste package model based on low level parameters and first principles would model each waste package individually and would require the following input:

- waste package inventories, elemental properties (e.g., solubilities) and decay chains;
- EBS and WP design characteristics;
- geological and hydrogeological characteristics;
- climatic variables; and
- definition and probabilities of disruptive event occurrences.

These parameters would then be input into and manipulated by physically based sub-models that would output higher level parameters (e.g., near field moisture and temperature characteristics). In the present model, however, the low-level physically based sub-models are not included (both because many of the necessary conceptual models and data do not currently exist, and because of the excessive computational time that would be required) and these sub-models are therefore "skipped". The higher level parameters therefore become required input parameters. As can be seen in Figure 3-14, some of these higher level parameters are dependent on some of the same lower level parameters. Although this dependency is not explicitly incorporated in the waste package model (since the low-level sub-models are not included), it should be implicitly incorporated during the process of developing subjective assessments of the high-level input parameters.

Conceptually, as more information becomes available, it may be possible in the future to replace some of the high-level input parameters with lower level parameters and their associated models that will output the higher level parameters directly.

3.4.1 Required Input Parameters

The required input parameters for the waste package model discussed above are summarized in greater detail below. These input parameters will be based on subjective assessments of experts, which, in turn, will be based on experimental data and more detailed modeling of some of the "lower-level" processes discussed above.

LEGEND

Input parameters required by present model

FIGURE 3-14
WASTE PACKAGE INPUT
PARAMETERS
ARGONNE/MODEL DEVELOPMENT

Recall that parameters can be specified as constants, stochastics, or functions. A constant parameter is assessed as a single value. A stochastic parameter is assessed not as a single value but as a distribution in order to represent the associated uncertainties. This distribution is sampled every system realization. Functions (i.e., dependent parameters) are described as a function of other parameters (which themselves may be either constant, stochastic or dependent).

The user may want to include a stochastic model error term as part of the definition of a dependent input parameter. For example, if k_{air} is described as a function of temperature, the following equation might be used:

$$k_{air} = f(TEMP) \times err_1 \quad (3.29)$$

where err_1 is the stochastic model error term.

Note that the following list supplies only a general description of the waste package model input parameters. A detailed description of the user interface and the actual manner in which these parameters are input is provided in the RIP User's Guide.

Waste Package Description. This data provides a general description of the characteristics of the waste package type(s) that are placed in the repository. *Each waste package type* is described in terms of the following parameters:

- number of waste packages
- MTIHM of waste per waste package
- effective waste burnup [MWd/MTIHM]

Note that the mass of waste in terms of MTIHM and the effective waste burnup are only required in order to normalize results to EPA limits in the manner specified by 40 CFR Part 191.

Near Field Environmental Conditions.

The behavior of the waste package is dependent on environmental conditions. Some of this dependency is explicitly included in the RIP computational algorithm (e.g., rewetting of waste packages after a thermal period). In addition, other parameters in the model can be described by the user as a function of specified environmental factors. Two environmental factors are automatically incorporated into the model: temperature and moisture conditions. They require the following input:

- the mean repository temperature history (in the rock)
- the incremental temperature history (above the mean repository temperature) at the edge of each different waste package type
- the uncertainty in the temperature histories specified above
- a description of the waste package-to-waste package variability about the mean temperature

- the temperature at which a waste package will rewet (i.e., revert to its long-term moisture condition)
- the fraction of waste packages in each of a number of user-defined *water contact modes* (after rewetting)

Note that the user can, if necessary, define other environmental parameters. These user-defined environmental parameters can also have a specified variability throughout the repository.

Radionuclide Inventory, Decay Chains, and Elemental Properties. This information must be provided for *every radionuclide in every type of waste package*:

- radionuclide name
- radionuclide specific activity (Ci/g)
- first order decay constant (yr^{-1})
- major daughter product
- radionuclide inventory [Ci/package]
- fraction of inventory that is classified as "free", "gap" and "bound"
- elemental solubility [g/m^3]
- effective diffusion coefficient [m^2/yr]
- is the element gaseous?
- partition coefficient for sorption inside the package [m^3/kg]

Waste Package Failure (Degradation).

Each waste package type is assigned by the user one or more failure modes for the primary containment layer (i.e., the outer waste package container). For each failure mode, the following information is required:

- a container failure distribution (failure rate vs. time) for the failure mode
- the probability of the failure mode being active in any given waste package
- the rate of aging (an acceleration/deceleration factor) for the failure distribution, which is typically described as a function of environmental factors

Each waste package is also assigned one or more failure modes for its secondary containment layer (i.e., the cladding for spent fuel; the pour canister for defense waste). For each of these failure modes, the following information is required:

- a container failure distribution (failure rate vs. time) for the failure mode
- the probability of the failure mode being active in any given waste package

Radionuclide Exposure Parameters.

Each waste package type requires specification of several exposure parameters. These parameters describe exposure of bound radionuclides (i.e., those radionuclides bound within the waste matrix) after failure of containment.

- the waste matrix aqueous alteration/dissolution rate [$\text{g/m}^2/\text{yr}$]
- the effective surface area of waste matrix (per unit mass) in a failed container [m^2/g]
- the effective fraction of surface area of waste matrix in a failed container that is wet (if desired, this parameter can be described as a function of container failure mode)
- the effective fractional air alteration rate of waste matrix [yr^{-1}]

Radionuclide Mass Transfer Parameters.

Each waste package type requires specification of several parameters that control mass transfer of radionuclides out of and away from failed containers.

- the groundwater flow rate at repository level for each waste package type [m/yr]
- the effective catchment area for flow, which determines the amount of water that actually comes into contact with waste matrix in a failed container (if desired, this parameter can be described as a function of container failure mode) [m^2]
- geometric factor for diffusive (aqueous) mass transport (if desired, this parameter can be described as a function of container failure mode) [m]
- volume of water contacting waste matrix in a failed container [m^3]
- mass of sorbent inside of waste package [kg]
- effective mass transfer rate for a gaseous radionuclide (must be specified for *each gaseous radionuclide*) [g/yr]

The final two categories of input couple the waste package component model to the radionuclide transport pathways component model and the disruptive events component model:

Waste Package Discharge Distribution.

Each radionuclide in each waste package type is assigned one or more discharge pathways. Mass released from the waste packages will be discharged to these radionuclide transport pathways. The data is entered as follows *for each discharge pathway*:

- name of the discharge pathway
- fraction of waste package release that is discharged to that pathway

Definition of radionuclide transport pathways is discussed in detail in Chapter 4.

Disruptive Events

- disruptive event definitions, probabilities, and consequences (discussed in detail in Chapter 5).

3.4.2 Model Output

The output of the waste package component model essentially consists of probabilistic waste package performance measures (e.g., cumulative release over time period of interest, maximum annual release). These measures can be examined for individual radionuclides, individual waste package groups, or summed over all radionuclides and all groups. Time histories of radionuclide release from the waste packages can also be produced.

The RIP User's Guide discusses the details of the various output options and how the data can be processed and graphically displayed (e.g., as a PDF, CDF or CCDF). As discussed in that document, the values of *all the input parameters for every realization* are also saved. This allows sensitivity analyses to be carried out in order to identify relationships between parameter values and performance.

The structure of the RIP model is such that the waste package component model can be run independently of the radionuclide transport pathways component model, producing the results outlined above. When the entire integrated model is run, additional outputs pertaining to the pathways component model are also produced (e.g., cumulative release to the accessible environment, peak individual dose). These outputs are discussed in Chapter 4.

3.5 Summary of the Waste Package Model

In order to properly apply this (or any) complex simulation tool, it is necessary to have a thorough understanding of the major assumptions on which the computational algorithm is based. The general outline of the waste package behavior model (presented in Chapter 2), highlighting the major model assumptions is reproduced below.

General Model Structure

- The waste package component model is part of the total system performance model, and is directly coupled to component models describing disruptive events and radionuclide transport pathways.
- The model is based on subjective assessments of relatively high level phenomenological parameters, such as container and cladding/pour canister failure distributions, and generalized alteration and mass transfer parameters.
- The model simulates groups of waste packages (rather than tracking the behavior of each of the individual waste packages in the repository).
- Waste package parameters can be described by the user as a function of temporally varying environmental conditions.
- The model incorporates radioactive decay and production of daughter products.

Environmental Conditions

- Temperature and moisture conditions are explicitly included in the model. The temperature at the edge of the waste package varies with time. Moisture conditions refer to the mode of water contact at a waste package (which are completely user-defined). Both temperature and moisture conditions can be specified as variable across the repository.
- Other environmental conditions (e.g., chemistry, stress) can be added by the user. Environmental conditions can be described as being spatially and temporally variable.
- A simple rewetting model is used that assumes that waste packages return to specified moisture conditions upon reaching a specified temperature. At temperatures above the specified temperature, the waste package is considered to be dry.

Waste Package Failure Rates

- Two levels of waste package containment (and failure) are explicitly simulated: the primary container (the waste package itself); and the secondary container (e.g., cladding for spent fuel, pour canisters for high level defense waste).
- Waste package failures are described in terms of density functions of failure frequency.
- Containers and cladding/pour canisters can fail by one or more failure modes. The model combines failure modes by assuming that the failures can be treated independently (they do not act with synergism).
- Container failure modes can be affected by temporally varying environmental conditions.

Mass Exposure

- Exposure of radionuclides is brought about by primary and secondary container failure, as well as matrix alteration/dissolution processes.
- The radionuclide inventory is made up of three additive components: the free inventory, which is exposed immediately upon primary container failure, the gap inventory, which is exposed immediately upon secondary container (e.g., cladding) failure in a failed container, and the bound inventory, whose exposure is controlled by alteration/dissolution of the waste matrix.
- Exposure of the bound inventory can be controlled by dissolution of the matrix and/or air alteration of the matrix. Dissolution is described in terms of a matrix

dissolution rate and an effective wetted surface area. Dissolution is zero prior to rewetting of the waste package.

- The effective wetted surface area of matrix can be described as a function of container failure mode. It is assumed that for a waste package that fails by more than one mode, the effects on wetted surface area are additive.

Mass Transfer

- For an aqueous radionuclide, mass transfer can be described as an advectively or a diffusively controlled process, each of which may be limited by radionuclide solubilities.
- Aqueous mass transfer is set equal to zero prior to rewetting of the waste package.
- Diffusive mass transfer can only be described in the waste package component model as a steady state process. The pathways component model can be appropriately used, however, to represent transient waste diffusive releases.
- Several mass transfer parameters can be described as functions of container failure mode. It is assumed that for a waste package that fails by more than one mode, the effects on mass transfer are additive.
- The mass transfer rate for gaseous species is directly specified by the user.

Effect of Disruptive Events

- Disruptive events can affect the behavior of the waste package. Disruptive events are simulated in a separate model component. Their consequences can manifest themselves in the waste package model in three ways: 1) a portion of the waste packages can be disrupted in place; 2) a portion of the waste packages (and their inventory) can be moved directly to the accessible environment or some other location; and 3) the parameters describing waste package behavior and/or environmental conditions may be changed.

Linkage to Transport Pathways Model

- The waste package model is coupled with the transport pathways model in two ways: 1) it relies upon the same large scale hydrologic parameters utilized and/or defined within the transport pathways component (e.g. repository level flow rate); and 2) each waste package type discharges its mass to a specified transport pathway (or pathways) defined by the user.

As noted previously, the fact that RIP simulates groups of waste package (as opposed to individual waste packages) is an approximation that has two effects: 1) it tends to overestimate mass transfer rates; and 2) it requires that mass transfer be independent of the time of container failure (although, as discussed previously, this can be compensated for by appropriately

defining transport pathways). Note that *conceptually*, modifying the model to simulate individual waste packages would not be difficult. It would, however, create a *computational* problem. That is, in order for such an approach to accurately represent variability throughout the repository, a large number of individual waste packages would need to be simulated, and this would be computationally intensive, severely limiting the practical use of the model. Due to the large amount of uncertainty in required input parameters, the effects mentioned above, which are introduced by not modeling waste packages individually, were deemed to be of secondary importance. This situation may change, however, as more experience is gained with waste package performance assessment, and future versions of RIP may include explicitly sampling and simulating individual waste packages.

Figure 3-15 expands on Figure 3-2 and represents a detailed waste package influence/information flow schematic. This diagram illustrates how the various input parameters and component models are linked together. It shows in detail how the various input and output parameters are moved between smaller component models to generate the waste package release distribution with time, graphically summarizing the structure of the waste package model.

Note that arrows connecting input parameters indicate that these parameters may be described as functions of other input parameters. For example, waste package failure mechanisms can be defined in terms of near field conditions. Likewise, disruptive events can affect near field conditions (which in turn may affect other input parameters).

3.5.1 Summary of Waste Package Computational Algorithm

A simplified summary of the computational algorithm for RIP, emphasizing the waste package portion of the model, is presented below in Figure 3-16.

FIGURE 3-15
 DETAILED WASTE PACKAGE
 INFLUENCE/INFORMATION FLOW
 SCHEMATIC
 ARGONNE/MODEL DEVELOPMENT

Begin nr = 1, number of Monte Carlo realizations

realize all non-temporal system parameters
realize all disruptive events over time period of interest

Begin t = 1, number of time steps

increment elapsed time
compute time-dependent variables
if disruptive event occurs, realize consequences

Begin j = 1, number of environmental groups

evaluate all parameters that depend on environmental factors

Begin n = 1, number of radionuclides

compute exposure rate
compute maximum mass transfer rate
compute release rate
release mass to specified pathways
update amount of exposed, unreleased mass
decay exposed, unreleased mass

end n loop

end j loop

decay radionuclides in waste packages
simulate radionuclide transport through pathways for this time step

end t loop

compute performance parameters for current realization

end nr loop

FIGURE **3-16**
WASTE PACKAGE MODEL
COMPUTATIONAL ALGORITHM
ARGONNE/MODEL DEVELOPMENT

3.6 List of Symbols

$c(t)$ -	total primary container failure modes at time t [1/t]
$c_m(t)$ -	container failure rate for failure mode m at time t [1/t]
$C(n)$ -	effective concentration at waste package for radionuclide n [M/L ³]
$C_s(n)$ -	saturation concentration of radionuclide n in water [M/L ³]
CATCH -	effective catchment area for a waste package [L ²]
CONTAC -	integer that is used to reference the water contact mode, each mode having been assigned a different value
$D_{eff}(n)$ -	effective diffusion coefficient for radionuclide n [L ² /t]
$D_m(n)$ -	molecular diffusion coefficient for radionuclide n in water [L ² /t]
$e(n,t)$ -	total exposure rate of radionuclide n for a group of waste packages at time t [M/t]
$e_f(n,t)$ -	exposure rate of radionuclide n in the free inventory for a group of waste packages at time t [M/t]
$e_g(n,t)$ -	exposure rate of radionuclide n in the gap inventory for a group of waste packages at time t [M/t]
$e_b(n,t)$ -	exposure rate of radionuclide n in the bound inventory for a group of waste packages at time t [M/t]
f_w -	fraction of waste matrix surface area in a failed container that is wet
$f_{w,m}$ -	fraction of waste matrix surface area that is wet due to failure mode m
$f_{free}(n)$ -	fraction of mass of radionuclide n in the "free" inventory
$f_{gap}(n)$ -	fraction of mass of radionuclide n in the "gap" inventory
FLOW -	repository level groundwater flow rate [L/t]
$g(t)$ -	rate at which matrix becomes unprotected [1/t]
i -	index referring to waste package type
$I_f(n,t)$ -	free inventory of radionuclide n <i>per unfailed container</i> at time t (that portion located between the cladding and the container wall) [M]

$I_g(n,t)$ -	gap inventory of radionuclide n <i>per unfailed container</i> at time t (that portion located in the gap between the fuel and the cladding) [M]
$I_b(n,t)$ -	bound inventory of radionuclide n <i>per unfailed container</i> at time t (that portion bound in matrix) [M]
$k_{a/d}$ -	combined fractional alteration/dissolution rate of waste matrix [1/t]
k_{air} -	fractional air alteration rate of waste matrix [1/t]
k_{wat} -	fractional aqueous alteration/dissolution rate of waste matrix [1/t]
$k_t(n,t)$ -	maximum possible mass transfer rate of radionuclide n out of and away from a group of waste packages at time t [M/t]
$k_{tp}(n)$ -	maximum possible mass transfer rate of aqueous radionuclide n out of and away from a single waste package [M/t]
$k_{tp,a}(n)$ -	maximum possible advective mass transfer rate of aqueous radionuclide n out of and away from a single waste package [M/t]
$k_{tp,d}(n)$ -	maximum possible diffusive mass transfer rate of aqueous radionuclide n out of and away from a single waste package [M/t]
$k_{tp,g}(n)$ -	maximum possible mass transfer rate of gaseous radionuclide n out of and away from a single waste package [M/t]
$k_{tp,m}(n)$ -	maximum possible mass transfer rate of aqueous radionuclide n out of and away from a single waste package due to container failure mode m [M/t]
m -	index referring to container and/or cladding failure mode
$M(n,t)$ -	amount of exposed (available) mass of radionuclide n in a group of waste packages at time t [M]
$M_p(n)$ -	amount of exposed (available) mass of radionuclide n per waste package [M]
$M_{uu}(t)$ -	fraction of mass that is unprotected, unaltered, and undissolved for a group of waste packages at time t
NM -	total number of primary container failure modes
n -	index referring to radionuclide type
N_c -	number of waste packages

N_m -	cumulative number of waste packages that have failed by mode m
N_T -	total number of waste packages that have failed by any mode
$r(n,t)$ -	release rate of radionuclide n from a group of waste packages at time t [M/t]
$R_{age}(m)$ -	aging rate for container failure mode m
R_{dis} -	matrix aqueous alteration/dissolution rate [M/L ² /t]
S -	effective surface area of waste matrix in a failed container per unit mass [L ² /M]
t -	time [t]
T_r -	temperature at which a waste package rewets, returning to its long term moisture condition [T]
t_{wet}	time at which a group of waste packages rewets [t]
$TEMPAV_i(t)$ -	the average temperature at the edge of waste package type i at time t [T]
$TEMPV$ -	parameter describing waste package to waste package temperature variability
$T_m(t)$ -	the mean temperature throughout the entire repository at time t [T]
$T_i(t)$ -	the incremental temperature above the mean repository temperature at the edge of waste package type i at time t [T]
V_w -	water volume in contact with matrix in failed waste package [L ³]
$V_s(n)$ -	equivalent volume in waste package due to sorption [L ³]
$w(t,\Theta)$ -	secondary container failure rate at time t for a primary container that has failed at time Θ [1/t]
Θ -	time of primary container failure [t]
τ -	dummy integration variable for time [t]
τ_D -	tortuosity for diffusive mass transfer
ω -	geometric factor for diffusive mass transfer [L]
η_e -	effective porosity

4. NEAR- AND FAR-FIELD RADIONUCLIDE TRANSPORT MODEL

As discussed in Chapter 2, the integrated repository performance assessment model RIP is a complex radionuclide transport model. RIP consists primarily of a series of inter-connected, fully coupled component models with input/output relationships for radionuclide transfer. The four major component models address: waste package behavior and radionuclide release; transport of radionuclides to the accessible environment through pathways; disruptive events; and fate and effect (dose or risk) in the biosphere.

This chapter discusses the transport of radionuclides through the near- and far-field to the accessible environment. The general methodology and assumptions incorporated in this component of the software are presented in detail. The RIP pathways component model is significantly different from transport models used in most other performance assessment computer programs. RIP attempts to *describe* rather than *explain* the processes controlling radionuclide transport. The rationale for choosing this approach is discussed in Chapter 2.

Section 4.1 describes how a pathway network is used to represent the geologic media, natural features (rivers, lakes, atmosphere, etc.) and man-made features (mines, boreholes, etc.) that comprise the environment at a repository site. Section 4.2 provides an overview of the computational algorithm used by the geosphere pathways model. The mathematical details of the algorithm are then presented in Section 4.3. Section 4.4 discusses the required input parameters for geosphere pathways. Section 4.5 discusses the biocell pathway algorithm. The pathway model output is described in Section 4.6. A summary is provided in Section 4.7. Section 4.8 contains a list of symbols referred to in this chapter.

4.1 Pathway Networks

The central feature of the transport model is the *pathway*. RIP uses pathways linked successively to one another to represent the physical process of radionuclide transport from the waste packages to the regulatory compliance point. (In U.S. legislation the regulatory compliance point is referred to as the *accessible environment* and that term is used frequently in this manual). The user can arrange pathways in series or parallel throughout the physical domain. Pathways can be used to describe water flow balance as well as radionuclide transport.

The RIP user defines pathways and their linkages and has complete discretion to define the number and complexity of pathways within the network. RIP pathways can be used to transport radionuclide mass in either the gas or liquid phase. Radionuclide exchange between phases is not possible within a single pathway, although the pathways may coexist in space. The pathways do not necessarily have to transport radionuclides. The user can construct pathways that do not receive mass, but interact with flow boundary conditions (e.g., precipitation) to provide subsequent pathways with consistent volumetric flow rates.

Figure 4-1 illustrates a few of these concepts with a *hypothetical* pathway configuration for the proposed Yucca Mountain High-Level Waste Repository. Please note that this figure and the associated discussion are presented only to illustrate features of the pathways component model and are not intended to represent the preferred conceptual model for the Yucca Mountain site.

Unsaturated Groundwater Flow

- (I) Tiva Canyon Member
- (II) Topopah Spring Member
- (III) Episodic Flow in Fractures

Gaseous Phase Transport

- (VIII) Region Above Repository

Flow and Transport

- (IV) Topopah Spring Member (Unsaturated Zone)
- (V) "Short Circuit Pathway" (Unsaturated Zone)
- (VI) Calico Hills (Unsaturated Zone)
- (VII) Prow Pass Member (Unsaturated Zone)
- (IX) Prow Pass and Bullfrog Member (Saturated Zone)

LEGEND

--- ▼ --- Water Table

FIGURE 4-1
**EXAMPLE PATHWAY CONFIGURATION
 FOR YUCCA MOUNTAIN**
 ARGONNE/MODEL DEVELOPMENT

The proposed repository is sited in the unsaturated Topopah Spring rock stratum within Yucca Mountain. There are unsaturated geologic strata above and below the repository. At depth, there is an aquifer that flows laterally away from the site. Rainfall on the mountain can potentially infiltrate the unsaturated strata, leach radionuclides from the repository and transport them to the aquifer. Once in the aquifer, they may move laterally until they reach the regulatory compliance point (accessible environment). Simultaneously, gaseous-phase radionuclides (primarily tritium) may seep upwards through the unsaturated zone and reach the accessible environment at the ground surface.

In Figure 4-1, pathways I and II represent infiltration of rainwater downward to the repository level. Neither pathway carries radionuclides. However, the computed water flow from these pathways is used to determine the volume of water that is leaching radionuclides from the repository. Pathway VIII represents upward advection of gaseous-phase radionuclides to the atmosphere. Pathway VIII coexists in space with pathways I and II (i.e., upward flow of gas can occur through the Topopah Spring and Tiva Canyon strata at the same time that rainwater is infiltrating these strata).

Pathway IV represents unsaturated aqueous flow from the repository through the matrix and fractures in the Topopah Spring stratum to the Calico Hills stratum. Pathway VI represents unsaturated aqueous flow from the Topopah Spring stratum through the Calico Hills stratum to the Prow Pass stratum. Pathway VII represents unsaturated aqueous flow from the Calico Hills stratum through the Prow Pass stratum to the aquifer in the Prow Pass and Bullfrog strata. Pathway V represents episodic saturated fracture flow (flow that may occasionally occur if a fracture becomes saturated) from the repository to the water table (Prow Pass and Bullfrog strata). Both pathways IV and V are used to model downwards aqueous phase transport. The two pathways coexist in space (both exist throughout the Topopah Spring stratum), but represent two different types of flow phenomena that could potentially occur in the same geologic stratum.

Thus, the pathways form a network with one pathway discharging into another. Pathway geometry is not rigidly defined in space, and it is possible for pathways to coexist in space. The network is a surrogate for physical transport phenomena that the RIP user considers to be of importance. The key features of the pathway network are the *connectivities* between pathways and user-defined *pathway parameters* that capture the behavior of the physical process. Figure 4-2 shows the pathway connectivities for the hypothetical Yucca Mountain example.

RIP provides two built-in types of pathway to represent transport within and between environmental media: *geosphere pathways* and *biocell pathways*. Most media can be represented using either type of pathway. Generally, geosphere pathways are used to represent subsurface hydrologic processes (such as fluid flow through an aquifer, or gaseous flow through rock). Biocell pathways are typically used to model transport between above-surface features (such as ponds, streams, and the atmosphere). The algorithms used to compute transport through geosphere and biocell pathways are described in Sections 4.2 and 4.5 respectively.

Unsaturated Groundwater Flow

- (I) Tiva Canyon Member
- (II) Topopah Spring Member
- (III) Episodic Flow in Fractures

Gaseous Phase Transport

- (VIII) Region Above Repository

Flow and Transport

- (IV) Topopah Spring Member (Unsaturated Zone)
- (V) "Short Circuit Pathway" (Unsaturated Zone)
- (VI) Calico Hills (Unsaturated Zone)
- (VII) Prow Pass Member (Unsaturated Zone)
- (IX) Prow Pass and Bullfrog Member (Saturated Zone)

LEGEND

---▼--- Water Table

FIGURE **4-2**
CONNECTIVITY OF YUCCA MOUNTAIN PATHWAYS
 ARGONNE/MODEL DEVELOPMENT

4.2 Overview of Geosphere Pathways Computational Algorithm

Within a pathway network, geosphere pathways are used primarily to model fluid (gas or liquid) flow through geologic media (soil and rock). This section describes in general terms how RIP geosphere pathways work.

4.2.1 Flow Modes

Large-scale heterogeneity in the hydrologic system (i.e., among different geologic media and geologic structures) is addressed by using multiple pathways to simulate radionuclide transport. Within a pathway, the user can address local hydrologic heterogeneity by using *flow modes*. For example, fracture flow and matrix flow through a rock mass could be two flow modes for a pathway. Homogeneous strata are typically modeled with only one flow mode.

Referring back to our Yucca Mountain example, pathway IV has two flow modes: unsaturated fracture flow and unsaturated matrix flow. The assumption implicit in this representation is that a droplet of water flowing through the Topopah Spring stratum will flow for some distance through a fracture. At some point, the fracture will terminate, at which point the water will flow through the matrix. The velocity at which flow occurs through the fracture will be different from the velocity at which flow occurs through the matrix. Also, there will be some *transition rate* that will characterize the frequency at which the water droplet will change mode from fracture flow to matrix flow. The transition rate will be some function of real physical properties of the rock, such as fracture spacing and length.

Pathway VII is used to represent saturated flow through the aquifer in the Prow Pass and Bullfrog strata. Pathway VII has only one flow mode despite the fact that both fracture flow and matrix flow can occur in these formations. In this case, it has been assumed that the majority of the flow occurs in the fractures. A retardation coefficient is used to capture the effects of aqueous diffusion into the rock matrix.

Each flow mode within a pathway has a defined set of hydrologic parameters:

- fraction of flow occurring in that flow mode;
- dispersivity (only used for single-flow-mode pathways);
- transition rate (only used for multiple-flow-mode pathways);
- velocity or porosity; and
- retardation coefficients.

RIP uses these parameters together with the pathway length to define a *breakthrough curve* for the pathway. RIP uses the calculated breakthrough curve to compute the mass transport rate for the pathway.

4.2.2 Breakthrough Curves

Within a geosphere pathway, RIP calculates radionuclide transport using a *breakthrough curve*, which is of the form shown in Figure 4-3. A breakthrough curve indicates the proportion of mass released from the pathway to a subsequent pathway as a function of time, based on a unit mass input at time zero (i.e., the time when mass first enters the pathway). RIP computes the breakthrough curve as a function of pathway length and the flow-mode hydrologic parameters (fraction of flow occurring in that mode; dispersivity; transition rate; velocity or porosity; and retardation coefficients). Because each radionuclide can have different retardation coefficients, RIP calculates breakthrough curves for each group of elements that has a unique set of retardation coefficients. The user can define each of the parameters as stochastic variables (i.e., as a probability distribution) to account for variability and uncertainty.

The breakthrough curve for a pathway combines the effects of all flow modes and retardation parameters on the radionuclide travel time. In single-flow-mode geosphere pathways, RIP computes the breakthrough curve using a one-dimensional advection-dispersion solution, as described in Section 4.3.1.1. In multiple-flow-mode geosphere pathways, RIP computes the breakthrough curve using an approximate Markov process algorithm, as described in Section 4.3.1.2. The Markov algorithm simulates a process whereby particles travel a certain length in a flow mode and then transition to another flow mode. This process continues until the particle exits the pathway, as shown on Figure 4-4. The likelihood, or probability, for a particle to be in a specific flow mode is directly related to the proportion of the total flow for the pathway occurring in the flow mode. For example, if most of the flow in a pathway occurred through the rock matrix, there would be greater chance at any given time that a particle would be in the matrix than in other flow modes of the pathway.

The RIP geosphere pathways algorithm uses a discretized form of the computed breakthrough curve to compute radionuclide mass transport. Each time step, RIP uses the discretized breakthrough curve for each pathway to calculate the percentage of the incoming mass that will be released in the following time step and for each subsequent time step. The incoming mass is thus discretized and released in appropriate amounts in subsequent time steps. The mathematical formulation of this algorithm is presented in Section 4.3.2.

4.2.3 Effect of Transient Changes and Disruptive Events on Radionuclide Transport

As discussed above, RIP computes the breakthrough curve as a function of the following parameters:

- pathway length,
- flow mode velocity or porosity,
- flow mode proportion of total fluid flow in the pathway,
- flow mode Poisson transition rate,
- dispersivity, and
- retardation factors

for example . . .

$$\frac{[U^{238}]_{out}}{[U^{238}]_{in}}$$

Cumulative
Proportion

Note: Cumulative proportion is less than one due to radioactive decay

FIGURE 4-3
EXAMPLE BREAKTHROUGH
CURVE FOR A RADIONUCLIDE
ARGONNE/MODEL DEVELOPMENT

FIGURE 4-4
**MARKOV PROCESS ALGORITHM
 FOR PARTICLE TRANSPORT
 ALONG A GEOSPHERE PATHWAY**
 ARGONNE/MODEL DEVELOPMENT

Consequently, if any of these parameters changes as a function of time, other conditions, or disruptive events, the breakthrough curve will also change.

When RIP recalculates the breakthrough curve for each radionuclide, RIP *does not* redistribute mass that is already in the pathway prior to the change in the breakthrough curve. RIP only distributes mass that enters the pathway subsequent to the change (and the mass generated by radioactive decay) using the new breakthrough curve.

Decreasing the pathway length affects more than the breakthrough curve. If the pathway length decreases (e.g., the length of an unsaturated zone pathway decreases because of a rising water table), RIP releases mass from the pathway to its defined discharge pathways in fractions equal to the fractional change in pathway length. For example, if the pathway shortens by 20%, then RIP would release 20% of the mass to the "downstream" pathway(s). Mass remaining in this pathway after this release is then lumped and redistributed according to the newly calculated breakthrough curve. If the length increases, there is no redistribution or release of mass, but RIP recalculates the breakthrough curve as described above.

Recalculating the breakthrough curve and redistributing mass increases the computational time required to run a RIP simulation. However, small changes in the breakthrough curve may have only a small effect on a simulation. This is particularly true if a path does not transport much mass or there is a lot of uncertainty in the flow parameters used to calculate the breakthrough curve. For example, travel time is inversely proportional to velocity. Consequently, a 1% change in flow-mode velocity will result in a change of approximately 1% in the expected travel time along the pathway. Considering the uncertainty in the travel time for the pathway, a 1% change may not be significant. To reduce computation time in the event of minor changes to the breakthrough curve, RIP allows the user to specify *tolerance values*. If breakthrough-parameters do not exceed the tolerance values RIP will not recalculate the breakthrough curve. Tolerance values are defined as minimum required fractional change in any of four parameters (pathway length, flow mode velocity or porosity, proportion of fluid flow in a given flow mode, and Poisson transition rate). If none of these parameters has changed sufficiently to exceed the tolerance value, RIP does not recalculate the breakthrough curve. (Note that there is no tolerance value for retardation or dispersivity. Changes to these parameters always result in recalculation of the breakthrough curve.) Of course, the user can set the tolerance value to zero to force recalculation of the breakthrough curve every time there is any change in any of these parameters. Section 4.4.1.4 discusses tolerance values in more detail.

4.2.4 Summary of Geosphere Pathways Computational Algorithm

The RIP user links individual pathways together into a network. Output from one pathway is input for one or more additional pathways. A *breakthrough curve* controls transport times for individual radionuclides through a given pathway. Each radionuclide in each pathway has a different breakthrough curve. The form of the breakthrough curve is a function of the flow-mode parameters. RIP computes the breakthrough curve using either a one-dimensional advection-dispersion solution or a Markov-process algorithm. RIP also computes radionuclide decay. Because of radioactive decay, the mass of a given radionuclide within a pathway may increase or decrease with time.

The parameters controlling radionuclide transport (e.g., flow mode velocities, transition rates, pathway lengths, radionuclide retardation) along a pathway may be dependent on a number of system parameters, including climate, disruptive events, hydrologic parameters, and flow system heterogeneity. Figure 4-5 shows the dependencies that affect the computational algorithm for transport through a single pathway.

Figure 4-6 summarizes how the algorithm outlined above is incorporated into the overall Monte Carlo scheme of RIP. The two major computational tasks carried out by the pathways model are:

- 1) computation of the breakthrough curves for each radionuclide in each pathway (based on pathway and flow mode characteristics); and
- 2) propagation of mass through the various pathways based on the shape of the breakthrough curves.

The mathematical details of these tasks are described in Section 4.3.

4.3 Mathematical Details of Geosphere Pathways Transport Algorithm

This section describes the mathematical details of the computational algorithm that RIP uses to calculate mass transport in geosphere pathways. Although these details may be of interest to the serious RIP user, they are not critical to achieving a broad understanding of the algorithm. The reader may therefore wish to skip directly to Section 4.4.

This section has been divided into two parts. The first deals with how the radionuclide breakthrough curve is calculated. The second shows how this breakthrough curve is used within RIP to transport mass.

4.3.1 Computing the Radionuclide Breakthrough Curve for a Geosphere Pathway

The two methods available in the RIP model for computing breakthrough curves are:

- 1) a solution to the advection-dispersion equation; and
- 2) the Markov process algorithm.

For either algorithm the breakthrough curves for a radionuclide are dependent on the RIP pathway and flow-mode parameters;

- pathway length
- pathway area
- flow rate
- retardation parameters
- Poisson rate parameters (for the Markov algorithm)

FIGURE 4-5
**OVERVIEW OF RADIONUCLIDE
 TRANSPORT PATHWAYS MODEL**
 ARGONNE/MODEL DEVELOPMENT

Begin nr = 1, number of Monte Carlo realizations

realize all non-temporal system parameters
realize all disruptive events over time period of interest

Begin t = 1, number of time steps

increment elapsed time
compute time-dependent variables
if disruptive event occurs, realize consequences

Begin j = 1, number of environmental groups

release mass from waste packages to pathways

end j loop

Begin k = 1, number of transport pathways

evaluate if parameter values have changed
if changed or t = 1 then
 compute breakthrough curve
 compute mass distribution coefficients
decay mass in each pathway cell
release mass to "downstream" pathway

end k loop

end t loop

compute performance parameters for current realization

end nr loop

FIGURE **4-6**
RADIONUCLIDE TRANSPORT MODEL
COMPUTATIONAL ALGORITHM
ARGONNE/MODEL DEVELOPMENT

The following two sections describe the solution methods in detail.

4.3.1.1 The Advection-Dispersion Algorithm

The advection-dispersion algorithm is the simplest and most commonly used transport mechanism within RIP. However, it has the limitation that it can only be used for pathways that have a single flow mode.

The algorithm used in RIP derives from the theoretical solution for one-dimensional transport in an infinite column with uniform flow of a tracer slug. The governing equation is presented below, and is discussed in detail in Bear (1979, page 266).

The idealization considers a thin slug of radionuclide particles which at $t=0$ are injected into an infinite column at location $x=0$. The partial differential equation governing solute distribution is given by;

$$\frac{\partial C}{\partial t} = D_h \frac{\partial^2 C}{\partial x^2} - \frac{q}{n} \frac{\partial C}{\partial x}, \quad -\infty < x < +\infty \quad (4.1)$$

where:

- C is the concentration of solute [M/L^3],
- t is the time [T],
- x is the distance from the injection location [L],
- D_h is the coefficient of hydrodynamic dispersion [L^2/T],
- q is the specific discharge [L/T], and
- n is the porosity [-].

The first term on the right hand side of Equation 4.1 considers transport due to dispersion, while the second term allows for transport with the average flux in the system.

If an observer moves in the positive x direction at the average advective flow rate, the distribution of mass within the pathway has the form illustrated in Figure 4-7 and the governing equation becomes;

$$\frac{\partial C}{\partial t} = D_h \frac{\partial^2 C}{\partial x'^2} \quad (4.2)$$

where

$$x' = x - \frac{q}{n}t \quad (4.3)$$

The initial conditions, $C=C(x,t)$, are in the form of a *Dirac delta function*, $\delta(x)$

$$C(x,0) = \frac{M}{n}\delta(x); \quad \delta(x) = \lim_{m \rightarrow 0} \delta_m(x) = \begin{cases} (1/m) & \text{for } 0 < x < m, m > 0 \\ 0 & \text{elsewhere} \end{cases}$$

$$M = \int_{-\infty}^{\infty} nC(x',t)dx' \quad (4.4)$$

and the value of $C(x,t)$ tends to zero as the absolute value of x' tends to infinity.

The solution to equation 4.2 is reproduced in Bear (1979, page 266) as;

$$C(x,t) = \frac{M}{n} \frac{1}{(4\pi D_h t)^{1/2}} \cdot \exp\left\{-\frac{(x - \frac{q}{n}t)^2}{4D_h t}\right\} \quad (4.5)$$

For input into RIP, the relationship between solute concentration and time is required in the form of a breakthrough curve; equivalent to the mass of solute that leaves a pathway of length L between specified time intervals. The mass of solute that leaves the pathway before time t is represented by the area under the curve (Equation 4.5 and Figure 4-7) between $x=L$ and $x=+\infty$. Therefore, between times t_i and t_{i+1} the mass of solute leaving the pathway per unit area of the pathway is given by:

$$\text{Change in mass per unit area} = [1-F(L, t_{i+1})] - [1-F(L, t_i)]$$

where $F(L,t)$ is the integral of Equation 4.5.

By inspection Equation 4.5 is seen to resemble the integrand of a Standard Normal Distribution;

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right\} \quad (4.6)$$

RIP therefore generates the breakthrough curve for advective-dispersive flow by integrating Equation 4.5.

FIGURE 4-7
**IDEALIZED PROGRESS OF SLUG FOR
 ADVECTION-DISPERSION ALGORITHM**
ARGONNE/MODEL DEVELOPMENT

4.3.1.2 The Markov Algorithm

RIP uses the Markov algorithm to model mass transport through multiple-flow-mode media. An example of multiple-flow-mode transport is dual porosity flow, in which a typical radionuclide is transported in a fracture, diffuses into the surrounding matrix, and then later returns to a fracture.

The multiple-state Markov process algorithm provides tremendous advantages in modeling. Use of multiple flow modes within a single pathway provides a powerful means of addressing local heterogeneity within a hydrologic unit. Conventional continuum-based algorithms have limited ability to address this. The Markov algorithm used in RIP is also far less numerically intensive than continuum transport models. This results in large savings in computing time making it practical to carry out large numbers of simulations.

However, the Markov algorithm also has some disadvantages. The Markov algorithm uses *descriptive* parameters (e.g., velocity, transition rate) rather than *physical* parameters (e.g., hydraulic gradient and hydraulic conductivity). Therefore, the RIP pathway algorithm approximates fluid flow behavior rather than modeling the physical process of fluid flow. For any complex system, the RIP user has to run other, more detailed models to develop an understanding of the flow pathways in order to define RIP input parameters. Also, the Markov process does not attempt to maintain a balance of fluid flow within the defined system of pathways. The responsibility is on the user to assign self-consistent flow parameters to achieve a balance of flow and maintain a physically reasonable system.

This sub-section first describes the Markov process algorithm and how RIP implements its approximation to the Markov process algorithm, and then describes how RIP computes multiple-mode breakthrough curves.

In the Markov process algorithm (and its implementation within RIP), the breakthrough curve for a radionuclide is a function of the pathway and flow mode parameters. The specific parameters on which the breakthrough curves depend are the pathway length, the proportions of flow occurring in each flow mode, the fluid velocities of the flow modes, the Poisson rate parameters, and the radionuclide retardation parameters. All of these parameters may be functions of time (or disruptive events). Therefore, the breakthrough curve may change with time during a simulation.

The Markov process algorithm has two steps. These are carried out repeatedly to simulate transport of a particle along a pathway. Step 1 consists of assigning the particle to a new flow mode. This assignment is a function of the proportions of flow occurring in the modes. Step 2 consists of propagating the particle a random length in the flow mode based on the Poisson rate parameter. In a random simulation, the outcome of step 1 is obtained by inverting the following conditional probability distribution:

$$\text{Pr}(\text{flow mode } j \mid \text{flow mode } i) = f_{Qj} / (1 - f_{Qi}) \quad (4.7)$$

where $\text{Pr}(\text{flow mode } j \mid \text{flow mode } i)$ is the probability of transition to flow mode j if previously in flow mode i , and f_{Qi} is the proportion of the total fluid flow occurring in the i th flow mode. The particle must move to a new flow mode, and therefore for a pathway with only two flow modes the probability of moving to the other flow mode is 1.

The relation between probability and flow mode is an assumption that is only valid if the proportions of flow in the flow modes remain constant over all infinitesimal lengths along the pathway. This implies that the same flow proportions apply to each discrete flow mode along the entire pathway.

Once assigned to a flow mode, RIP calculates the random length traveled by a particle using a Poisson distribution, given by:

$$l = -\frac{1}{\lambda_j} \ln[r(0,1)] \quad (4.8)$$

where:

- l is the random length interval [L];
- λ_j is the Poisson transition rate from flow mode j [1/L] per unit length of pathway ; and
- $r(0,1)$ is a random number between 0 and 1.

Equation 4.8 is based on the inverse of the exponential probability distribution (Benjamin and Cornell, 1970).

Given average linear fluid velocities for the flow modes, RIP converts the random length traveled by a particle in a flow mode to a travel time. The total travel time over the pathway is the sum of all travel times along the individual flow mode intervals. By repeating the particle simulation procedure a large number of times, we can numerically approximate the probability distribution for travel time through the pathway. RIP directly equates this distribution to the breakthrough curve.

Figure 4-8 illustrates two trivial examples for a two mode system in which dispersion has been neglected. Mode 1 represents fracture flow and is associated with a short travel time. Mode 2 represents matrix flow and the travel time associated with this flow mode is slower. In the first curve the Poisson transition rate for all flow modes is very small; implying that the particle travels a large distance before a transitioning between flow modes. Therefore, only a few radionuclides change modes and we observe two distinct breakthroughs (Figure 4-8a). In the second curve the Poisson transition rate for all flow modes is large; implying most particles only travel a short distance before transitioning to the other flow. In this example we cannot distinguish the individual flow modes within the breakthrough curve (Figure 4-8b) and the majority of the particles break through at an "average" travel time. The average travel time is

calculated from the "average" velocity, given by $\sum (\text{Velocity in flow mode } i \times \text{Proportion of flow in flow mode } i)$.

Figure 4-9 illustrates the form of the breakthrough curve for a more realistic three-mode system. Note that particles cannot travel faster than the fastest mode, nor slower than the slowest. As seen observed in the previous example, the effect of some particles covering the entire path length in a single mode is to introduce "steps" into the breakthrough curve. However, variation about the mean travel time for modes 1 and 2 produces a smoother breakthrough curve.

In the RIP model, an approximation to the Markov process algorithm (Cox and Miller, 1965) reduces the quantity of computational work that must be performed. In the approximate Markov process algorithm, particles travel only their first random length in an individual flow mode. Subsequently, a particle travels any remaining length of the pathway at the expected (average) velocity of all the flow modes. This approximation retains the steps in the breakthrough curve associated with a radionuclide traveling the entire pathway in a single mode and is generally adequate for simulations with large uncertainty in the flow mode and pathway parameters. However, the errors introduced may be unacceptable for the rare situations where flow mode parameters are well defined.

Using this approximation the travel time for a particle is given by the following:

$$t_n = \left[l_i / V_i + (L_p - l_i) \sum_j^N f_{Q_j} / V_j \right] R_n \quad (4.9)$$

where:

- t_n is the travel time for radionuclide n [T];
- l_i is the initial length interval traveled in flow mode i [L];
- V_i is the average linear fluid velocity for flow mode i [L/T];
- L_p is the pathway length [L];
- N is the number of flow modes in the pathway,
- f_{Q_j} is the proportion of the total fluid flow occurring in pathway j ,
- V_j is the average linear fluid velocity for flow mode j [L/T]; and
- R_n is the retardation parameter for radionuclide n .

The first term on the right side of Equation 4.9 is the travel time along the initial length interval of flow mode i . The second term on the right side of Equation 4.9 is the travel time over the remaining length at the expected (average) velocity.

- (a)** Low Poisson Transition Rate
- (b)** High Poisson Transition Rate

FIGURE **4-8**
EXAMPLE OF 2-MODE SLUG
INPUT WITHOUT DISPERSION
 ARGONNE/MODEL DEVELOPMENT/WA

3-Flow Modes

t_i = flow mode travel time ($i=1,2,3$)
 $\bar{t}$ = expected travel time

FIGURE 4-9
 APPROXIMATE MARKOV PROCESS ALGORITHM
 EXAMPLE BREAKTHROUGH AND DENSITY PLOTS
 ARGONNE/MODEL DEVELOPMENT

In the approximate Markov process algorithm, some fraction of particles may travel the entire path length in each individual flow mode (as illustrated by the "spikes" in the probability density function in Figure 4-9). Equation 4.9 is formulated to directly account for the fraction of particles that may traverse the pathway relatively quickly, in comparison to the average travel time.

The benefit of the approximate Markov process algorithm is that the breakthrough curve has a closed form solution, thus, RIP can calculate the breakthrough fractions for each directly. This direct calculation for the breakthrough curve is as follows:

$$F_n(t) = \sum_j^N f_{Qj} J_{jn}(t) \quad (4.10)$$

where:

- $F_n(t)$ is the probability for radionuclide n to have a travel time less than t ,
- N is the number of flow modes in the pathway,
- f_{Qj} is the proportion of flow in the j th flow mode, and
- $J_{jn}(t)$ is the probability for radionuclide n after starting in flow mode j to have a travel time less than t .

Equation 4.10 is the sum over the pathway flow modes of the intersection of two events. The first event is that a particle started traveling in mode j and has probability f_{Qj} . The second event is that the particle's travel time was less than t and has probability $J_{jn}(t)$.

The mode probability distribution, $J_{jn}(t)$, is discontinuous. It requires several decision steps that are functions of the flow mode fluid velocity relative to the pathway average fluid velocity. For a given travel time, t , the mode probability distribution is given by:

$$J_{jn}(t) = \begin{cases} 0, & \text{for } t \leq \frac{L_p}{V_j} R_n < \bar{t} \\ 1 - F_j(l_j), & \text{for } \frac{L_p}{V_j} R_n < t < \bar{t} \\ 1, & \text{for } \frac{L_p}{V_j} R_n < \bar{t} \leq t \\ 0, & \text{for } t \leq \bar{t} < \frac{L_p}{V_j} R_n \\ F_j(l_j), & \text{for } \bar{t} < t < \frac{L_p}{V_j} R_n \\ 1, & \text{for } \bar{t} < \frac{L_p}{V_j} R_n \leq t \end{cases} \quad (4.11)$$

where:

- L_p is the pathway length,
- V_j is the fluid velocity for the j th flow mode,
- R_n is the retardation parameter for radionuclide n ,
- $\bar{t}$ is the average travel time for the pathway, and
- $F_j(l_j)$ is the exponential probability distribution for length intervals traveled in flow mode j

RIP computes the average travel time for the pathway from the following:

$$\bar{t} = L_p R_n \sum_j^N \frac{f_{Qj}}{V_j} \quad (4.12)$$

The length parameter, l_j , which is an argument to $F_j(l_j)$ in Equation 4.9, is obtained by solving Equation 4.11 for l_j . This solution is given by:

$$l_j = L_p \left[\frac{t - \bar{t}}{\frac{L_p}{V_j} R_n - \bar{t}} \right] \quad (4.13)$$

where the parameters used in Equation 4.12 and Equation 4.13 are defined in Equation 4.11. The first three conditions in Equation 4.11 apply to flow modes in which the travel time for a particle remaining in the flow mode for the entire pathway (given by $R_n \cdot L_p/V_j$) is less than the

pathway average travel time ($\bar{t}$ from Equation 4.12). The last three conditions apply to flow modes for which the individual mode travel time is greater than the average travel time.

The reader will find comparisons of the approximate and exact Markov process algorithms in Appendix H. Visual comparison of selected parameter sets show the comparisons are generally favorable, although, in certain cases considerable error occurred. The range of the error was generally within a factor of 3 and included both under- and over-estimation of the travel time by the approximate method. If the pathway and flow mode parameters have high uncertainty, this error will not add significantly to the total error and will cause no harm to the analysis. If uncertainty in the pathway and flow mode parameters is low (which will typically be very unlikely), use of the approximate method will have greater impact on the analysis and may be inadequate for the simulations.

4.3.2 Radionuclide Mass Propagation Algorithm for Geosphere Pathways Transport

In geosphere pathways, RIP uses the breakthrough curve to evaluate what fractions of the total input to the pathway exit the pathway over different time periods. Because there is a separate breakthrough curve for each radionuclide, RIP also calculates the mass transport separately for each radionuclide.

In the algorithm, the pathway is represented as a single row of "cells" or "bins". Each cell has its own *residence time*, which is length of time it will hold the mass before discharging it to the next pathway. RIP distributes the incoming mass to the cells in proportions that are based on the breakthrough curve. The mapping of the breakthrough curve onto the cells for a pathway is shown on Figure 4-10 and described below. These "cells" essentially serve as mass buffers and the reader should not consider them to have spatial significance.

RIP assigns the *residence times* as follows:

$$2^{i-2} \Delta t < \delta t_i \leq 2^{i-1} \Delta t \quad (4.14)$$

where:

δt_i is the residence time for cell i ; and

Δt is the RIP time step interval (e.g., 100 years).

The following table below shows how RIP would assign cells and residence times for a 10,000 year simulation, based on time steps of 10, 50 and 100 years, respectively. Note that the residence time of the last cell exceeds the total simulation time.

FIGURE 4-10
**MAPPING OF BREAKTHROUGH CURVE
 ONTO GEOSPHERE PATHWAY CELLS**
 ARGONNE/MODEL DEVELOPMENT

	$\Delta t = 10$ years	$\Delta t = 50$ years	$\Delta t = 100$ years
cell	Pathway Entry Residence Time (years)	Pathway Entry Residence Time (years)	Pathway Entry Residence Time (years)
1	0 - 10	0 - 50	0 - 100
2	10 - 20	50 - 100	100 - 200
3	20 - 40	100 - 200	200 - 400
4	40 - 80	200 - 400	400 - 800
5	80 - 160	400 - 800	800 - 1600
6	160 - 320	800 - 1600	1600 - 3200
7	320 - 640	1600 - 3200	3200 - 6,400
8	640 - 1,280	3200 - 6,400	6400 - 12,800
9	1,280 - 2,560	6400 - 12,800	12,800 - 25,600
10	2,560 - 5,120	12,800 - 25,600	
11	5,120 - 10,240		
12	10,240 - 20,480		

As discussed in Section 4.3.1, RIP develops the breakthrough curve by computing the cumulative proportion of the total mass that is released from the pathway as a function of time (referred to as $F(t)$). $F(t)$ approaches 1.0 as t increases (i.e., the cumulative proportion of the mass that has been released increases over time; at some time in the future all the mass will have been released and at that time $F(t) = 1$). Furthermore, $F(t) - F(t-1)$ is equal to the fraction of the mass released between $t-1$ and t . The breakthrough curve is mapped onto the pathway cells by computing $F(t)$ for the time associated with the beginning and end of each cell. For example, assuming a 10 year time step, if the computed breakthrough curve indicated that 30% of the mass was released by $t = 640$ and 42% by $t = 1280$, 12% (42%-30%) of the mass entering the pathway would be mapped onto cell #8.

Each cell is emptied every $2^{i-2} \Delta t$ years. RIP empties the contents of Cell 1 each time step to the next pathway downstream. The contents of other cells are redistributed when emptied. For example, Cell 2 is emptied every time step to Cell 1; Cell 3 is emptied every other time step, with half its contents moving to Cell 2, and half moving to Cell 1; Cell 4 empties every third time step, with half its contents going to Cell 3, and one-quarter going each to Cells 1 and 2. Cell 5 empties every fourth time step, half its contents going to Cell 4, one quarter to Cell 3 and an eighth to Cells 2 and 1. This results in a smooth release of mass. For example, mass entering

Cell 6 at year 0 is released in equal amounts between years 160 and 320 (assuming $\Delta t = 10$ years) to the next downstream pathway.

The use of cells is an approximation of the true breakthrough curve. The effects of the approximation can be illustrated with a few examples. First, consider the case of 1 gram of mass being released, instantaneously at year zero, to a pathway with a theoretical travel time of 200 years and no dispersion. Assuming a 10 year time step, RIP assigns the entire 1 gram of mass to Cell 6, and releases it uniformly between 160 and 320 years. With a 50 year time step, the entire 1 gram of mass is assigned to Cell 4, and released uniformly between 200 and 400 years. This is illustrated in Figure 4-11, which compares the RIP solutions for mass transfer with analytic solutions for mass transfer. Note that, with this algorithm, RIP may predict *initial* breakthrough times that are less than or equal to theoretical breakthrough time, but *never* greater than the theoretical time.

Figure 4-12 further illustrates mass transfer within RIP for the case of a continuous 1 gram/year source of mass, with no dispersion. Note that when using a 10 year time step, RIP predicts breakthrough at 160 years, while with the 50 year time step RIP perfectly matches the theoretical breakthrough curve.

Figure 4-13 and 4-14 repeat the examples shown in Figure 4-11 and 4-12, but include the effect of dispersion. Again RIP predicts early breakthrough for the point source of mass, but approximates the shape of the mass transfer curve quite closely. The RIP approximation for a continuous source of mass and dispersion is even better (Figure 4-14). Also, notice that after the first couple of 100 years, the RIP predictions using 50 and 100 year time steps are identical. This is because 100 years is a factor of 2 greater than 50. Thus, after 100 years, these two simulations have cells with identical residence times, as shown in the table above. This illustrates an important feature of the algorithm used in RIP: the use of coarser time steps does not result in large penalties in terms of algorithm precision. Instead, the precision of the algorithm depends on the manner in which the pathway is discretized into "bins" or "cells". It is anticipated that future versions of RIP will allow the user to change the manner in which the cells are defined.

While radionuclides reside in a pathway cell, they undergo radioactive decay and daughter-product generation. RIP simulates this process at every time step. The radioactive decay algorithm is discussed in detail in Appendix D.

In the RIP model, the radionuclide masses in each cell are simultaneously decayed and decay series are accounted for. However, RIP *does not* redistribute the daughter product to the pathway cells until they are released from the cell of the parent. That is, daughter products remain in the cell of the parent until the release time and are not distributed (i.e., they move at the same speed of their parent until they leave the pathway). This incurs some error for those daughter products that have significantly different retardation characteristics than the parent. This error can be minimized by adding discretization to the pathways (i.e., making the pathways shorter).

Cumulative Mass Transport Single Instantaneous Source (1 gram)

Mass Transport Rate Single Instantaneous Source (1 gram)

— Analytic Solution
+ RIP - 10 yr timestep
o RIP - 50 yr timestep

FIGURE 4-11
SLUG INPUT WITH NO DISPERSION
ARGONNEMODEL DEVELOPMENT

Cumulative Mass Transfer

Continuous Mass Input (1 gram/year)

Breakthrough Curve

Continuous Mass Input (1 gram/year)

- Analytic Solution
- + RIP - 10 yr timestep
- ◊ RIP - 50 yr timestep

FIGURE 4-12
CONSTANT INPUT WITH NO DISPERSION
ARGONNE/MODEL DEVELOPMENT

Cumulative Mass Transfer Single Instantaneous Source (1 gram)

- Analytic Solution
- + RIP - 10 yr timestep
- ◊ RIP - 50 yr timestep
- ▲ RIP - 100 yr timestep

Mass Transport Rate Single Instantaneous Source (1 gram)

FIGURE 4-13
SLUG INPUT WITH DISPERSION
ARGONNEMODEL DEVELOPMENT

Cumulative Mass Transfer

Continuous Mass Input (1 gram/year)

- Analytic Solution
- + RIP - 10 yr timestep
- ◊ RIP - 50 yr timestep
- ▲ RIP - 100 yr timestep

Breakthrough Curve

Continuous Mass Input (1 gram/year)

FIGURE **4-14**
CONSTANT INPUT WITH DISPERSION
 ARGONNE/MODEL DEVELOPMENT

4.4 Defining Input Parameters for the Geosphere Pathways Transport Algorithm

4.4.1 General Description of Required Input Parameters

This section provides general documentation on the meaning of input parameters used to define radionuclide transport. Additional documentation is provided in the RIP User's Guide.

Pathway input parameters can generally be divided into the following categories:

- 1) bulk pathway parameters;
- 2) pathway discharge parameters;
- 3) pathway flow mode parameters; and
- 4) tolerance values for transient parameters.

These data categories are discussed below.

4.4.1.1 Pathway Bulk Parameters

The user must enter the following parameters for each pathway defined:

- pathway identification;
- pathway description;
- pathway length [L];
- pathway total volumetric flow [L^3/T];
- pathway total area [L^2].

The pathway identification and description are constant values. The description is for user reference. The identification may be used elsewhere, such as when defining the discharge of a subsequent pathway. The pathway length, total volumetric flow, and total area all have the potential to be either constant, stochastic (i.e., random variables), or functions of other defined parameters, including the simulation time. Pathway volumetric flow and pathway area do not affect the breakthrough curve if the user selects *velocity* as the flow-mode descriptor parameter; the input velocity is used directly. If the user selects *porosity* as the flow-mode descriptor parameter, RIP uses volumetric flow, flow area, and the porosity value to calculate a pathway velocity, which is in turn used in the breakthrough curve calculation.

4.4.1.2 Pathway Discharge Parameters

Each pathway may discharge radionuclide mass to other pathways or to the accessible environment. The user must enter two parameters per discharge pathway. These are:

- discharge pathway identification
- mass fraction of remaining mass discharged to the pathway

The pathway identification is the user-defined identification for the target pathway. RIP uses the fraction of remaining mass to determine the proportion of mass to be discharged from the current pathway to the target pathway. Because RIP determines this proportion based on the remaining (unallocated) mass, the order in which the user defines discharge pathways is important. The mass fraction parameter may be either constant, stochastic, or a function of other parameters. RIP allocates mass based on the remaining fraction of mass to ensure that the total fraction of mass allocated sums to exactly 1, even when the user defines mass allocation parameters as stochastic variables. The proportion of mass allocated to a given pathway can be different for different radionuclides if desired.

4.4.1.3 Flow Mode Parameters

The user can represent local heterogeneity in the fluid flow field of a pathway with flow modes. There may be up to five flow modes for a pathway. Each flow mode is defined by the following RIP input parameters:

- flow mode description;
- fraction of pathway total volumetric flow rate;
- velocity or porosity (user preference) [L/T] or [];
- Poisson transition rate (see below) [L^{-1}];
- dispersivity [L];
- radionuclide retardation parameters.

As stated previously, the RIP pathways component model is significantly different from transport models used in most other performance assessment computer programs. RIP attempts to *describe* rather than *explain* the processes controlling radionuclide transport. The parameters required by RIP to describe flow reflect this philosophy. RIP requires parameters like velocity, which are a function of the conditions in the flow system rather than inherent characteristics of the flow system.

Because these descriptive parameters are a function of flow-system conditions, the user will typically define them as functions of other parameters that RIP does not require as input. For example, the user could define fluid velocity as a function of hydraulic conductivity, and hydraulic gradient. RIP does not require the user to enter values for hydraulic conductivity or hydraulic gradient, but the user could define them as parameters to construct the dependency. Chapter 2 presents more detailed information concerning the definition of "sub-models" such as these.

The flow-mode description is a text field for user definition of the flow mode. The user can enter the remaining parameters as constants, stochastics, or functions of parameters. It is only possible to enter either the velocity or porosity because the two parameters are dependent on one another as follows:

$$v_i = \frac{f_{Qi} Q}{A n_i} \quad (4.15)$$

where:

- v_i is the average linear fluid velocity for the i th flow mode,
 f_{Qi} is the fraction of the pathway volumetric flow rate occurring in the flow mode i ,
 Q is the total volumetric flow rate for the pathway,
 A is the total area normal to the flow direction for the pathway, and
 n_i is the effective porosity for the i th flow mode.

The user can enter a Poisson transition rate for only one flow mode in a pathway. RIP computes the remaining transition rates based on the given transition rate and the fraction of flow in each mode. This is discussed further in Appendix G. RIP does not use the Poisson transition rate if the pathway has only one flow mode.

If the pathway has only one flow mode, RIP uses velocity and dispersivity to solve the one-dimensional advection-dispersion equation (Bear, 1979, page 266). Neglecting molecular diffusion, the hydrodynamic dispersion term of this relation is:

$$D_{Hi} = |V_i| \alpha_i \quad (4.16)$$

where:

- D_{Hi} is the hydrodynamic dispersion coefficient for flow mode i ,
 V_i is the average linear fluid velocity of the i th flow mode, and
 α_i is the longitudinal dispersivity for the i th flow mode.

The approximate Markov process algorithm does not use dispersivity.

The user enters radionuclide retardation parameters on a group basis for each flow mode of a pathway. The radionuclide groups consist of suites of radionuclides whose retardation parameters are similar. The group classifications simplify the user input. The user defines them in the Waste Package module of the RIP model. Each radionuclide group may have separate retardation parameters for sorption and matrix diffusion. RIP combines these parameters into a single retardation value as shown in Appendix I. The combined retardation value remains constant for the simulation.

4.4.1.4 Tolerance Values

A tolerance value is the minimum fractional change required for a parameter value before RIP recalculates a pathway breakthrough curve. Thus, although a parameter may change, RIP will not recalculate the breakthrough curve until the magnitude of the change exceeds the tolerance value. This can reduce computation time during a simulation. The tolerance values specified by users remain constant for each simulation.

The RIP user must specify tolerance values for five parameters. RIP uses these tolerance values for *all* pathways and all flow modes. The tolerance values required by the RIP model are the following:

- pathway length tolerance
- flow proportion tolerance
- fluid velocity tolerance
- porosity tolerance
- Poisson transition rate tolerance

Only the first parameter, pathway length, is a bulk pathway parameter. The remainder are flow mode parameters. The user defines the tolerance value in terms of the fractional difference between a new value and the old value of the specified parameter. RIP computes this fractional difference as follows:

$$\Delta p = \frac{|p^{\text{new}} - p^{\text{old}}|}{\text{MIN}(p^{\text{new}}, p^{\text{old}})} \quad (4.17)$$

where:

Δp is the fractional difference for parameter p ,

p^{new} is the new value for parameter p , and

p^{old} is the old value for parameter p .

RIP compares the fractional difference Δp , to the user-specified tolerance value to determine whether the breakthrough curve should be recalculated. If Δp does not exceed the tolerance value, RIP does not recalculate the breakthrough curve and does not update p^{old} . The user can specify $\Delta p=0$ and thus force recalculation of the breakthrough curve every time there is a change in any of these parameters.

In determining the tolerance values, the user must consider the importance of changes in the parameters. For example, travel time is inversely proportional to velocity. Consequently, a 1% change in the flow-mode velocity results in a change of approximately 1% in the expected travel time along the pathway. Considering the uncertainty in the travel time for the pathway, the user must decide if the 1% change is significant.

4.4.2 Managing the Water Balance

The long-term release of radionuclides from a repository system can be strongly dependent on the groundwater flow rate at the repository level (see Chapter 3). The actual quantity of flow contacting waste at the repository level is governed by the quantity of flow available and the hydraulic properties of the intervening geologic media. Likewise, the flow available to transfer mass from the repository through the geosphere is governed by these same parameters.

The RIP program does not force the user to maintain a water balance amongst the pathways. For example, if two pathways discharge into a third pathway, the volumetric flow rate in the third pathway does not have to be equal to the sum of the discharges from the two preceding pathways. The inherent assumption here is that if the flows do not sum, it is because the RIP user knows of an additional source (or sink) of flow that does not warrant explicit modeling. This has the advantage of computational efficiency but does make it possible for the user to define a physically unreasonable flow system.

The user can define a flow balance by specifying pathway total volumetric flow rates consistent with mechanics of the flow system being modeled. The user should specify pathway volumetric flow rates with dependencies on one another such that flow at the repository level and elsewhere in the simulation domain is consistent with the flow volumes entering at the boundaries of the domain.

In constructing the flow balance, users may wish to define pathways that do not transport radionuclide masses (e.g., pathway III in Figure 4-1). Such pathways could include a precipitation/infiltration model and account for the hydraulic properties of the intervening strata.

4.5 Biocell Pathways Transport Algorithm

As discussed at the beginning of the chapter, the transport pathways algorithm propagates radionuclide mass along a network of interconnected *geosphere pathways* and *biocell pathways*. Geosphere and biocell pathways are alternate models used by RIP to represent transport within and between environmental media. The previous sections have dealt in detail with geosphere pathways. In this section, we describe biosphere pathways.

Most media can be represented using either type of pathway. Generally, geosphere pathways are used to represent subsurface hydrologic processes (such as fluid flow through an aquifer, or gaseous flow through rock), while biocell pathways are typically used to model transport between above-surface features (such as ponds, streams, and the atmosphere).

A small lake probably provides the best physical analog for a RIP biocell. A lake is generally fed by streams or aquifers (in RIP terminology, pathways) and water entering the lake from a stream becomes mixed with water already in the lake. A lake also typically has a discharge stream (or streams). Given the lake's volume and the flow rate from the discharge stream(s), one can calculate a turnover time for the lake. Turnover time is the time it would take for the discharge streams to drain the lake at their given flow rate assuming no flow into the lake.

Alternatively, knowing the discharge time one could define outflow from the lake as fractional turnover rate (fractional turnover rate = $1/[\text{discharge time}]$) multiplied by the lake volume. This is the approach adopted by RIP in a biocell pathway. RIP makes the further assumption that any mass entering the lake (biocell) mixes instantaneously and completely throughout the lake (i.e., the concentration of mass in the biocell is uniform and reaches equilibrium instantaneously). The mathematics of this representation are discussed below.

Turnover rate is expressed as the fraction of mass leaving the biocell pathway per unit time. Thus, if there is no new mass added to the system, the current mass in the biocell pathway at any given time would be described by the expression:

$$m = m_o \cdot e^{-\lambda t} \quad (4.18)$$

where:

- m = current mass in cell [M];
- m_o = initial mass [M];
- λ = turnover rate [1/T]; and
- t = time [T]

Of course, mass may enter the biocell pathway from another pathway (geosphere or biocell) or directly from the waste packages at the same time that mass is exiting. RIP assumes that mass input occurs uniformly over a computational time step. Also, it is assumed that as soon as mass arrives in the biocell pathway, it is immediately available for transfer out of the cell, and that the incoming mass is transported out at the same rate as mass that was in the cell at the beginning of the time step (i.e., mixing is complete and instantaneous).

Given these assumptions, the following differential equation describes the mass rate of change for a single biocell:

$$\frac{dm_i}{dt} = \left[\sum_j m_j \lambda_j f_{ji} \right] + q_i \quad (4.19)$$

where:

- m_i = mass in biocell i [M];
- λ_i = turnover rate (fractional discharge rate per unit time) for biocell i [1/T];
- f_{ji} = fraction of discharge from biocell j that goes to biocell i ($f_{ii} = -1$; $0 \leq f_{ji} \leq 1$ for $j \neq i$); and
- q_i = rate of addition to biocell i from waste packages or geosphere pathways.

In matrix form, this can be expressed as follows:

$$\underline{M} = \underline{T} \underline{M} + \underline{Q} \quad (4.20)$$

where:

$$\underline{M} = \begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ . \\ . \\ . \end{bmatrix} \quad (4.21)$$

$$\underline{T} = \begin{bmatrix} \lambda_1 f_{11} & \lambda_2 f_{21} & \lambda_3 f_{31} & . & . & . \\ \lambda_1 f_{12} & \lambda_2 f_{22} & \lambda_3 f_{32} & . & . & . \\ \lambda_1 f_{13} & \lambda_2 f_{23} & \lambda_3 f_{33} & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{bmatrix} \quad (4.22)$$

and

$$\underline{Q} = \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ . \\ . \\ . \end{bmatrix} \quad (4.23)$$

In order to solve this system of equations, we apply the fully implicit (backwards difference) finite difference approximation:

$$\underline{M}(t) = \frac{(M(t) - M(t - \Delta t))}{\Delta t} \quad (4.24)$$

where Δt is the computational time step.

RIP carries out radioactive decay calculations asynchronously, by decaying the mass in a biocell at the end of the time step.

4.6 Pathways Model Output

The output of the pathways component model essentially consists of probabilistic performance measures (e.g., cumulative release *to* the AE or *from* a specific pathway over time period of interest, peak individual dose resulting from an exposure due to a particular pathway). These measures can be examined for individual radionuclides or summed over all radionuclides and all groups. Time histories of radionuclide release and dose can also be produced.

The RIP User's Guide discusses the details of the various output options and how the user can process and graphically display the data (e.g., as a PDF, CDF or CCDF). As discussed in the User's Guide, RIP saves the values of *all the input parameters for every realization*. This allows the user to carry out extensive sensitivity analyses to identify relationships between parameter values and performance.

4.7 Summary

The near- and far-field radionuclide-transport algorithm for the RIP model is based on a network of user-defined pathways. The pathways of RIP reflect major features of the biosphere and the hydrologic system. Pathways may represent large-scale heterogeneities of the geologic system, such as faults or formation scale stratigraphy, or other features such as lakes and streams. The user can address local heterogeneity within a geosphere pathway by defining multiple flow modes. The flow modes are primarily distinguished from one another based on flow velocity in the mode. However, flow modes may also conduct varying proportions of the total pathway flux, and use different radionuclide retardation parameters.

Within individual geosphere pathways, RIP uses a breakthrough curve to compute radionuclide transport. The breakthrough curve for a pathway combines the effects of all flow modes and retardation parameters on the radionuclide travel time. In single-flow-mode geosphere pathways, RIP computes the breakthrough curve using a one-dimensional advection-dispersion solution. In multiple-flow-mode geosphere pathways, RIP computes the breakthrough curve using an approximate Markov process algorithm. Mass transport in biocell pathways is much simpler, depending primarily on a user-defined turnover rate.

In a single-mode geosphere pathway, RIP computes the breakthrough curve using a one-dimensional advection-dispersion solution, as described in Section 4.3.1.1. For pathways consisting of more than one flow mode, RIP computes the breakthrough curve using an approximate multiple-state Markov-process algorithm, as described in Section 4.3.1.2.

4.8 List of Symbols

C	Concentration of the solute [M/L ³].
D _{Hi}	Hydrodynamic dispersion for flow mode <i>i</i> in a pathway [L ² /T].
f	Geometric factor for pathway cell residence times.

$F_n(t)$	Breakthrough curve value for radionuclide n at time t .
f_{Qi}	Fraction of pathway fluid flow occurring in the i th flow mode.
α_i	Dispersivity for flow mode i in a pathway [L].
λ_j	Poisson transition rate for the j th flow mode of a pathway [L^{-1}].
λ	Turnover rate for a biocell pathway [t^{-1}].
$J_{jn}(t)$	Cumulative probability distribution for travel time of radionuclide n in flow mode j .
l_i	Initial length traveled by a radionuclide in flow mode i [L].
L_p	Pathway length [L].
M	Mass of tracer injected into system [M].
m	Current mass in a biocell pathway [M].
m_0	Initial mass in a biocell pathway [M].
n	Porosity [-].
Δp	Fractional change in parameter p .
p^{new}	New value for parameter p .
p^{old}	Old value for parameter p .
q	Specific discharge [L/T].
$r(0,1)$	Uniformly distributed random number between 0 and 1.
R_n	Retardation parameter for radionuclide n .
σ	Standard deviation.
$\bar{t}$	Average travel time for a particle in a pathway [T].
Δt	RIP time step interval (e.g., 100 years) [T].
δt_i	Residence time for pathway cell i [T].
$t_{l,j}$	Left endpoint for time interval about pathway cell j [T].
t_n	Travel time for radionuclide n along a pathway.

$t_{r,j}$	Right endpoint for time interval about pathway cell j [T].
μ	Mean value.
V_i	Average linear fluid velocity for flow mode i [L/T].
w_{in}	Mass distribution coefficient for pathway cell i and radionuclide n .
x	Distance from the injection location [L].

5. DISRUPTIVE EVENTS COMPONENT MODEL

5.1 Introduction

The purpose of this chapter is to describe the structure of the disruptive events component model. This model modifies the behavior of the other main components models within RIP; the waste package behavior and radionuclide release model, the transport pathways model, and the risk/dose model. The chapter presents a review of the general methodology and assumptions incorporated into RIP, and discusses the application of the disruptive events component model to typical situations.

RIP defines a disruptive event as an occurrence that modifies other parameters values in RIP.

As discussed in Chapters 3 and 4, RIP is structured so that the RIP user can simulate transport pathways and waste package behavior independently. Each of these two modules produces a separate set of output results. In contrast, the disruptive events module only acts to modify other component models, and therefore is not structured to be run independently. Because the disruptive events module acts to modify the behavior of the other modules, it is recommended (although not essential) that the reader acquire an understanding of the manner in which waste package behavior and transport pathways are simulated in RIP prior to reading this chapter.

Section 5.2 explains what is meant by a "disruptive event" and provides an overview of the disruptive events modeling approach. Section 5.3 describes how disruptive event *occurrences* are selected and defined. Section 5.4 then specifically describes how disruptive event *consequences* are defined. Section 5.5 summarizes the disruptive events computational algorithm. Section 5.6 provides a summary discussion of the required disruptive event input parameters. Finally, Section 5.7 contains a glossary of terms used throughout Chapter 5.

5.2 Overview of Disruptive Events Methodology

The RIP integrated performance assessment model explicitly incorporates two types of uncertainty:

- Parameter uncertainty. The parameters describing the behavior of the repository system under a specified set of present and future conditions are uncertain.
- "Disruptive events". Future events are uncertain. "Disruptive events" may occur that change conditions and influence system parameters.

RIP explicitly includes the first type of uncertainty in the waste package model, transport pathways, and dose/risk models. RIP does this by treating the model parameters representing these processes as uncertain (i.e., representing them as distributions that are randomly sampled each Monte Carlo system realization). Examples of uncertainty that RIP treats explicitly in the waste package and transport pathways models are *processes* such as container corrosion, heating

and cooling of the waste packages, failure of borehole walls, and migration of radionuclides through fractures or faults.

The RIP model represents the second type of uncertainty using the disruptive events component model described in this chapter. *Disruptive events* are defined here as discrete perturbations of the repository system. That is, disruptive events are discrete occurrences that have some quantifiable effect on other processes and/or parameters within the RIP model. Note that discrete is a relative term, and does not necessarily imply instantaneous. Given the long time scales of interest (10,000 years or more), something taking place over a period of 100 years could be considered a discrete event. Examples of disruptive events include volcanism, faulting, and human intrusion. In general, the disruptive events component model is intended to represent relatively rare occurrences. Events that occur continuously throughout the time period of interest are generally more efficiently modeled as processes within the other component models.

It is noteworthy that climate change is not typically treated as a disruptive event. This is because climatic changes usually occur both gradually and continuously. It is therefore unusual for the process to be well represented by a discrete change in the RIP representation of the system. Typically the user would model climatic change (and the corresponding changes in environmental conditions such as water table elevation and infiltration rate) explicitly in the transport pathways and waste package behavior components.

There are two general approaches for analyzing the uncertainties described above (NRC, 1990). The first approach (referred to here as "simulation") consists of incorporating all uncertainties directly into the models and data bases describing the repository system. The second consists of developing and separately simulating "scenarios", which explicitly represent alternative ways in which the repository environment might change in the future. Each scenario may require a different conceptual and computational model for simulating the performance of the repository system. Most analyses use a combination of the two approaches (e.g., Bertram-Howery et al., 1990). The differences between the approaches are not severe, and both can be designed to produce results that are essentially equivalent. A more detailed discussion of the two approaches is presented in Appendix B.

The RIP model uses the "simulation" approach and explicitly incorporates all uncertainties directly into the component models and parameters, using a Monte Carlo method to sample parameters describing both processes and events. That is, RIP creates a time history of disruptive events (and other system parameters) for each Monte Carlo system realization of repository performance. Because RIP describes model parameters stochastically, each realization produces a different time history of events and processes. The integrated model is designed so that it can simulate all combinations of model parameters and time histories that might be realized.

As described below, a given disruptive event will be associated with one or more consequences. That is, a disruptive event has specific effects on waste package behavior and/or radionuclide transport in pathways or biosphere. These consequences can be treated stochastically. For example, if a certain disruptive event disrupts a number of waste packages (i.e., instantly failing

container and cladding), the actual number of waste packages affected could be a stochastic parameter.

Figure 5-1 schematically summarizes the relationships between RIP's four component models and its model parameters. The left side of the figure represents the two types of uncertainty. The first type, parameter uncertainty, is represented by the stochastic model parameters that control the waste package behavior, transport pathways, and dose/risk models. The second type of uncertainty, events, is represented by the disruptive events model, which can directly affect the other three component models and/or their parameters. Note that the disruptive events model also has stochastic input parameters.

The following three sections describe the selection and description of the disruptive events, specification of disruptive event consequences, and a summary of the computational algorithm by which the occurrences and consequences are incorporated into the integrated model.

5.3 Selection and Description of Disruptive Events

The set of all conceivable disruptive events that could occur at a potential geologic repository is illustrated in Figure 5.2. Only a small portion of these events can be considered credible, where a *credible event* is defined as an event possessing a significant probability of occurrence at the site over the time period of interest. According to the current U.S. regulations (40 CFR, Part 191, Appendix B), performance assessments need not consider events or processes that are estimated to have less than one chance in 10,000 of occurring over 10,000 yrs (i.e., an occurrence rate of 10^{-8} yr⁻¹).

Likewise, only a portion of the conceivable events at any given site can be considered to be *events of consequence* with respect to the performance of the repository. As illustrated in Figure 5-2, the disruptive events of interest are formed by the intersection of these two groups: those events that are both credible *and* of consequence. These are referred to here as *significant events*. It is the significant events that should be explicitly considered by the disruptive events model.

Identification of a complete set of significant events is a critical data input requirement for a RIP model. The process by which a complete set of significant events can be identified is discussed in detail by others (e.g., Cranwell et al., 1990; Guzowski et al., 1990).

RIP assumes that all disruptive events can be simulated as Poisson processes. This implies that the events occur singly and independently, and the probability that an event will occur in a short time interval is proportional to the length of the interval (Cox and Miller, 1965).

The assumption of independence of events is not strictly accurate in all cases. The occurrence of some events (e.g., faulting) may be related to the time period since a faulting event last occurred. Although the model could be modified to handle such a dependence, given the various uncertainties involved in the input parameters, a Poisson representation is considered adequate for the present purposes.

FIGURE 5-1
REPRESENTATION OF UNCERTAINTY IN RIP
ARGONNE/MODEL DEVELOPMENT/WA

FIGURE **5-2**
SET OF ALL CONCEIVABLE DISRUPTIVE EVENTS
ARGONNE/MODEL DEVELOPMENT/WA

The Poisson process is described by a single parameter, λ , the rate of occurrence, which has units of time⁻¹. λ is the expected number of occurrences per unit time.

The probability that x events will occur during a time interval Δt is given by the following expression:

$$\frac{e^{-\mu} \mu^x}{x!} \quad (5.1)$$

where

$$\mu = \lambda \Delta t \quad (5.2)$$

The Poisson distribution also has the property that the intervals between events are independently distributed with the exponential probability density function:

$$\lambda e^{-\lambda t} \quad (5.3)$$

In the RIP model, each event is defined by an *occurrence parameter* (i.e., an identifier for that particular event). The value of the occurrence parameter is internally computed by the model every time step during each system realization as a function of the rate of occurrence. This parameter takes on a value of 1 if the event has occurred during the current time step and a value of 0 if it has not (based on Equations 5.1 through 5.3).

RIP allows the user to specify that a particular event can, by definition, only occur once (i.e., it may not make sense physically for the event to occur more than once). The event is still represented by a Poisson process, but only two states are defined in any given realization at a given time: either the event has occurred, or it has not occurred. Once the event occurs, it is not allowed to reoccur.

RIP includes disruptive events to allow the user to model discrete occurrences. Therefore, in addition to defining how often an event may occur, the user typically assigns each disruptive event one or more *descriptor parameters*. Descriptor parameters are *stochastic* parameters that define the characteristics and magnitude of the event. These parameters are defined by the user for each disruptive event and are realized (i.e., a specific parameter value is randomly chosen from its distribution) whenever a disruptive event occurs. They are intended to be descriptive parameters that define the event, and can be used to quantify event consequences. For example, the descriptor parameters for a human intrusion/drilling disruptive event might be the number and depth of boreholes drilled. For a volcanic event, the descriptor parameters might include the length and width of the dike. The disruptive event consequences described in the following section will typically be functions of the sampled descriptor parameters.

5.4 Specification of Disruptive Event Consequences

RIP allows the user to specify the consequences of disruptive events in two ways:

- by describing the magnitude of a specific set of internally-defined (i.e., hard-wired into the model) discrete responses; and
- by explicitly identifying model parameters (describing waste package behavior and/or radionuclide transport through pathways and biosphere) that are functions of disruptive event occurrence and descriptor parameters.

The first type of consequence represents discrete responses to the event, such as the disruption of some waste packages. The second type of consequence represents *long-term effects* on the repository system (e.g., changing the hydraulic gradient in the saturated zone, raising the water table, opening a new transport pathway).

Each of these two types of consequences is described in detail below.

5.4.1 Discrete Response Consequences

For each disruptive event, there are four types of internally-defined disruptive event consequences that describe discrete responses:

- 1) *The radionuclides in a number of waste packages are moved directly to the accessible environment.* It is assumed that the inventory released from each package is equal to the inventory of an unfailed container at the time of the event. The consequence parameter is the number of waste packages affected.
- 2) *The radionuclides in a number of waste packages are moved directly to a specified pathway (e.g., the saturated zone).* It is assumed that the inventory released from each package is equal to the inventory of an unfailed container at the time of the event. It is also assumed that all of the waste package's inventory is immediately released to the pathway (i.e., the waste package is completely disrupted during the movement and the contents are not limited by any alteration, dissolution, or mass transfer processes at the waste package). The consequence parameters are the number of waste packages affected, and the pathway to which they are discharged.
- 3) *A number of waste packages are disrupted in place.* It is assumed that the cladding (or pour canister) instantaneously fails with the container. The consequence parameter is the number of waste packages disrupted. The exact manner in which this consequence is implemented in the RIP algorithm, and the resulting approximations involved, are discussed in detail in the RIP User's Guide.
- 4) *A portion of the mass (previously released from the waste packages) contained within a pathway is immediately discharged to another pathway or the accessible environment.* The

consequence parameters are the mass fraction discharged from each selected pathway.

The consequence parameters mentioned above may be represented stochastically. Furthermore, they can be described as functions of the descriptor parameters. For example, the number of waste packages disrupted by a drilling event could be described as a function of the number of boreholes. Of course, if a particular event does not produce one of the consequences outlined above, the appropriate consequence parameter is set to zero.

5.4.2 Consequences That Modify Waste Package and Transport Pathways Parameters

In addition to the four consequences described above, which are explicitly included in the model, it is also possible to directly influence parameters defined in the waste package, transport pathways, and dose/risk modules. This capability can be used to specify long-term consequences. A general discussion of the manner in which model parameters can be directly modified by disruptive events is summarized below. The precise manner in which the user can specify this dependence requires an understanding of the user-interface software, and is described in detail in the RIP User's Guide.

The user interface was designed to specifically incorporate user-defined sensitivities to disruptive events when defining parameter values. In particular, for any independent parameter (i.e., a parameter that is not described as a function; either a stochastic or a constant), the user can directly specify the parameter's sensitivity to specific disruptive events. The user defines how the current value of the parameter is to be modified should a particular disruptive event occur. The parameter is modified by a user-defined *influence parameter*, that can either *replace*, *multiply*, or be *added* to the original parameter value. This influence parameter may, in turn, be defined as a function of event descriptor parameters.

This capability is best illustrated by example. Suppose a magmatic intrusion disruptive event (represented by the *occurrence parameter* MAGMA) creates a dike that increases the hydraulic gradient in a saturated zone transport pathway (represented by the transport pathways model parameter GRADSZ). Assume that the user specifies that the magnitude of the gradient change is proportional to SIZE, which is a *descriptor parameter* for the magmatic intrusion disruptive event, describing the size of the magmatic intrusion (the constant of proportionality being 0.001).

The user could define the sensitivity of GRADSZ as follows:

if disruptive event MAGMA occurs, modify GRADSZ such that
$$\text{GRADSZ} = \text{GRADSZ} + \text{MAGMOD}, \text{ where } \text{MAGMOD} = 0.001 \times \text{SIZE}$$

MAGMOD is the user-defined *influence parameter*, described here as a function of the descriptor parameter SIZE. GRADSZ would retain the modified value for the remainder of the realization. If a second magmatic intrusion (or any other event that affected GRADSZ) occurred at a later time in the realization, RIP would once again update the value of. Note that SIZE is realized every time a magmatic event occurs.

5.5 Disruptive Events Computational Algorithm

A simplified summary of the computational algorithm for RIP, emphasizing the disruptive events portion of the model is presented in Figure 5-3.

Within the loop of Monte Carlo realizations, the algorithm steps through time simulating waste package behavior and radionuclide transport pathways. If an event occurs during a given time step, event descriptor parameters, event consequence parameters, and event influence parameters are realized, and affected system parameters are modified prior to simulating waste package behavior and transport through pathways for the time step.

At the end of the simulation time, the performance parameters for the current realization (e.g., cumulative release to accessible environment) are computed and saved. The algorithm then returns to the beginning of the loop and simulates another system realization. As discussed in Chapter 2, after an appropriate number of system realizations are simulated, the results are combined (e.g., into a CCDF) and analyzed.

RIP allows the user to change event occurrence rates during a simulation. This may be implemented in two different ways: 1) the rate of occurrence could be described as a function of time; and 2) the rate of occurrence could be modified by another disruptive event. Figure 5-3 shows how this is handled by RIP. At the beginning of the realization, the time of the first occurrence of each type of event is computed (based on the specified Poisson rate). Whenever an event occurs, the time interval until the next occurrence is computed. Furthermore, at the beginning of each time step, RIP checks to see if the rate of occurrence for any event has been changed. If it has, the time interval until the next event is recomputed.

It is important to understand that whenever a rate of occurrence is modified, *the next occurrence time is specified as the current time (i.e., the time at which the rate was modified) plus the newly computed time interval until the next event occurrence*. For example, if the original rate of occurrence was 0.0002 yr^{-1} (about once every 5000 years), and the rate of occurrence was modified at time = 4900 (which could be prior the first occurrence) to 0.000192 yr^{-1} (about once every 5200 years), it is quite possible that the Poisson distribution assumption will result in the event never occurring during a 10,000 year simulation, even though the occurrence rate throughout the simulation was never less frequent than once every 5200 years.

5.5.1 Monte Carlo Sampling Algorithm

Completely random Monte Carlo sampling could require a very large number of system realizations to statistically represent the range of system parameters and event occurrences, and this could prove to be computationally prohibitive. The RIP model, therefore, is structured to carry out the Monte Carlo sampling in an intelligent manner to increase efficiency. As pointed out in Section 5.1, RIP explicitly incorporates two types of uncertainty: 1) uncertainty regarding the parameters describing the behavior of the repository system under a specified set of expected present and future conditions; and 2) uncertainty regarding the occurrence and consequences of disruptive events that change conditions and influence system parameters.

Begin nr = 1, number of Monte Carlo realizations

realize all non-temporal system parameters
compute time interval to first occurrence for each event

Begin t = 1, number of time steps

increment elapsed time
compute time-dependent variables
if an event's rate of occurrence has changed, compute time interval to next occurrence

if an event has occurred during this time step, then:

realize event descriptor parameters
realize discrete response consequences
modify affected system parameters
compute time interval to next occurrence

simulate waste package behavior and transport through pathways, and
decay mass for this time step

end t loop

compute performance parameters for current realization

end nr loop

FIGURE **5-3**
DISRUPTIVE EVENTS
COMPUTATIONAL ALGORITHM
ARGONNE/MODEL DEVELOPMENT

Bias towards realizations in which events occur, and realizations at the extremes of the input distribution

FIGURE 5-4
**IMPORTANCE SAMPLING OF
 PARAMETERS AND EVENTS**
 ARGONNE/MODEL DEVELOPMENT/WA

Both of these uncertainties can be sampled in a biased manner (using importance sampling) to reduce the number of realizations required.

This is illustrated schematically in Figure 5-4, which shows the set of all possible futures for the repository system. The RIP Monte Carlo sampling algorithm can be intentionally biased towards realizations in which disruptive events occur, and realizations at the extremes of the input distributions. The results of the realizations sampled in this manner are subsequently weighted in an appropriate manner before they are combined. This produces better resolution of the high-consequence, low probability "tail" of the results distributions. This can be combined with a stratified (Latin-Hypercube) sampling approach to further improve the efficiency. The importance (and stratified) sampling algorithms are discussed in detail in Appendix C.

5.6 Summary of Required Input Parameters

The first, and perhaps most difficult task in attempting to simulate disruptive events at a repository is to develop a list of events that are both credible and of consequence with respect to repository performance. As discussed in Section 5.3 the selection procedure must be designed such that the completeness of the set can be demonstrated as far as that is possible

Once this list has been developed, the RIP model requires specific input for each defined event. The required input for describing the disruptive events is straightforward and is summarized below.

- *Rate of occurrence for disruptive event.* This represents the expected number of occurrences per unit time.
- *Can the event reoccur?* A particular event can be specified such that it can, by definition, only occur once.
- *Event descriptors.* These are user-defined parameters that are intended to be descriptive parameters that define the event, and can be used to quantify event consequences. For example, the descriptor parameters for a human intrusion/drilling disruptive event might be the number and depth of boreholes drilled.
- *Discrete response consequences.* There are four discrete response consequences defined by the model. These describe instantaneous, discrete consequences of the disruptive event:
 - 1) the number of waste packages whose contents are immediately moved directly to the accessible environment.
 - 2) the number of waste packages whose contents are immediately moved directly to a specified pathway (i.e., the saturated zone).
 - 3) the number of waste packages that are immediately disrupted in place.

- 4) the fraction of the mass in any specified pathway (e.g., the unsaturated zone) that is immediately discharged to another pathway or the accessible environment.

Note that these responses can be defined as functions of event descriptors.

- *Long-term consequences.* Long-term consequences of the event can also be defined. These are specified by defining the sensitivity of selected model parameters to disruptive events in terms of an influence parameter. If the particular event occurs, the user-defined influence parameter can replace, multiply or be added to the original parameter value. Model parameters that could be affected by disruptive events might include the hydraulic gradient in saturated zone, the water table elevation, or the fraction of mass released from waste packages that is partitioned into a given transport pathway. Like the discrete response consequences, the long-term consequences can also be defined as a function of event descriptors.

Specifying input for the disruptive events component model is discussed in more detail in the RIP User's Guide.

5.7 Disruptive Events Glossary

<i>consequence parameter</i>	- a parameter that describes the magnitude of one of a specific set of four internally-defined discrete instantaneous responses to a disruptive event.
<i>credible event</i>	- an event possessing a significant probability of occurrence over the time period of interest.
<i>descriptor parameter</i>	- a user-defined parameter that provides a description (quantification, characterization) of a disruptive event, and can be used to quantify event consequences.
<i>disruptive event</i>	- discrete perturbations of the repository system that have some quantifiable effect on waste package behavior and/or transport of radionuclides.
<i>influence parameter</i>	- a user-defined parameter that replaces, is added to, or multiplies a specified parameter value when a disruptive event occurs. This provides a means for representing long-term effects of disruptive events.
<i>occurrence parameter</i>	- the identifier for a disruptive event that automatically takes on a value of 1 or 0 depending on whether the event has occurred during the present time step.
<i>system realization</i>	- simulation of the repository system given a value (or time history) for each parameter and event occurrence.

scenario - an explicit representation of an alternative way in which the repository might perform in the future.

significant event - an event that is both credible and of consequence with respect to repository behavior. It is the significant events that are explicitly considered by the disruptive events model.

6. DOSE/RISK COMPONENT MODEL

The previous chapters of this manual describe how RIP models the release of radionuclides from the waste package, and how the released mass is transported through the geosphere and the biosphere. To this point RIP has been dealing with radionuclide *masses*. While modeling release and transport of radionuclides is important in its own right, it does not tell us directly about the effect of the release on human health. This chapter describes the general concepts of dose and risk, and how they can be modeled using RIP.

Section 6.1 first introduces the general concepts of dose and health risk. Section 6.2 then describes how doses are computed within RIP. Section 6.3 describes how doses are converted into health risk. Finally, Section 6.4 briefly describes the type of dose/risk results that can be saved by RIP.

6.1 Radionuclide Concentration and Health Risk

Health risk is assessed on the basis of the total radioactive *dose* received by people (receptors). Dose results from radionuclide uptake due to direct and indirect ingestion, inhalation, immersion, or contact with radionuclides present in various components of the environment. Examples of direct uptake include:

- Ingestion of water (ground water or surface water) containing radionuclides.
- Inhalation of contaminated air (including gaseous, airborne and dustborne radionuclides).
- Immersion in radioactive clouds
- Immersion (baths, showers, swimming) in contaminated water
- External exposure (contact) with contaminated soil

Indirect uptake of radionuclides largely results from ingesting food products (edible animal products, edible plants, marine and freshwater foods) that have themselves been in direct or indirect contact with radionuclides present in the environment. For example:

- Edible plants cultivated in contaminated soil, or irrigated with contaminated water.
- Livestock fed with contaminated feed or water.
- Fish culled from contaminated lakes, rivers, or oceans.

Dose is thus a complex function of radionuclide concentration in various environmental compartments. Dose is receptor specific. For examples, farmers are more likely to come into contact with contaminated soil while fishermen are more likely to come into contact with contaminated water. Also, dietary habits (and thus ingestion levels) are variable among different population groups. Dose is also radionuclide specific: some radionuclides are more

active than others; some radionuclides have a greater tendency to accumulate in the flesh of livestock.

In addition, health risk due to a given dose level may also be receptor specific. For example, a sub-lethal dose that poses a carcinogenic threat would be a greater risk to children than the elderly, because children are more likely to live long enough for the cancer to manifest itself.

6.2 Modeling Dose with RIP

The first step in defining a dose/risk model is to define the *receptor groups* who may potentially be exposed to the doses. A receptor group may be defined quite generally (e.g., all individuals living near the site) or quite specifically (individual fishermen between the ages of 20 and 40 living near the site). Note, however, that as mentioned above, many of the parameters of a dose/risk model are receptor specific, and therefore need to be specified such that they are consistent with the definition of the receptor group.

Average annual dose to an individual in receptor group g can be represented by the following expression:

$$D_g = \sum_j \sum_r D_{rjg} = \sum_j \sum_r DF_{rjg} \cdot C_{rj} \quad (6.1)$$

where:

- D_g = annual effective dose equivalent to a member of receptor group g from all radionuclides present in all pathways. Units must be consistent with radionuclide concentration (e.g., Sv/yr).
- D_{rjg} = annual effective dose equivalent to a member of receptor group g from radionuclide r present in pathway j (Sv/yr).
- C_{rj} = concentration of radionuclide r present in pathway j (g/m^3 or g/kg).
- DF_{rjg} = dose factor for receptor group g , pathway j , and radionuclide r . The dose factor is the dose received per unit concentration of radionuclide present in a pathway (e.g., $[\text{Sv}/\text{yr}]/[\text{g}/\text{m}^3]$ or $[\text{Sv}/\text{yr}]/[\text{g}/\text{kg}]$)

The dose factors (DF_{rjg}) for the various receptors as a function of radionuclide and environmental component (geosphere or biocell pathway) provide the only link within RIP between radionuclide concentrations and dose to receptors. Modeling of dose within RIP is thus very simple: for each defined receptor group, the annual dose is the sum of the concentration of each radionuclide in each environmental compartment multiplied by the appropriate dose factor. The RIP pathways component model calculates radionuclide concentration in each of the environmental components, and dose factors are input by the user as either constants, stochastics or functions. These products are summed to calculate the total dose to the receptor.

Appendix J discusses in general terms how a table of dose factors would be derived for input into RIP.

6.2.1 Calculation of Radionuclide Concentrations

RIP tracks transfer of radionuclide *mass* through the system being modeled. As discussed above, however, for dose modeling, radionuclide *concentrations* are required.

6.2.1.1 Concentrations in Geosphere Pathways

For a geosphere pathway, the concentration of radionuclide r , in pathway j , is calculated as follows:

$$C_{rj} = \frac{M_{rj}}{\sum_{i=1}^n (V_{ji} \cdot R_{jri})} \quad (6.2)$$

where:

- C_{rj} = concentration of radionuclide r in pathway j [M/L^3];
- M_{rj} = mass of radionuclide r in pathway j [M];
- V_{ji} = pore volume of pathway j , flow mode i [L^3]; and
- R_{jri} = retardation factor for radionuclide r in pathway j , flow mode i .

Equation 6.2 essentially represents the mass of radionuclide divided by the of the total pore volume available over all flow modes. The retardation term in the equation accounts for the fact that not all radionuclides are mobile (due to sorption and/or matrix diffusion). The equation assumes that the radionuclide concentration is equal in all flow modes (i.e., equilibrium has been achieved).

The pore volume of an individual flow mode is calculated as:

$$V_{ji} = L_j A_j n_{ji} \quad (6.3)$$

where:

- L_j = pathway length [L];
- A_j = pathway area [L^2]; and
- n_{ji} = effective porosity [-] for flow mode i of pathway j .

As discussed in Chapter 4, in a given flow mode, the user can specify the effective porosity, in which case the calculation above is performed directly, or the user may specify flow velocity, in which case the effective porosity is calculated using the following expression:

$$n_{ji} = f_{ji} Q_j / (A_j v_{ji}) \quad (6.4)$$

where:

$$\begin{aligned} Q_j &= \text{pathway volumetric flow [L}^3\text{/T];} \\ f_{ji} &= \text{fraction of pathway flow occurring in mode } i; \text{ and} \\ v_{ji} &= \text{average linear fluid velocity in mode } i \text{ [L/T].} \end{aligned}$$

Since the concentration computed for a pathway is determined by the volume over which mass in the system is averaged, larger (e.g., longer pathways) will tend to result in lower concentrations (and hence doses). This implies that when computing doses in geosphere pathways, it is best to discretize the pathways into short lengths. It is important, however, not to make the pathway too short. In particular, *the pathway length should be such that the transit time through the pathway for the fastest radionuclide is no less than one computational time step*. This requirement is necessary since RIP does not allow mass to move through a pathway in less than a time step. Specifying an extremely short pathway can therefore result in computed masses and concentrations that are artificially high.

6.2.1.2 Concentrations in a Biocell Pathway

For a biocell pathway, concentration is calculated as follows:

The concentration in solution is given by;

$$C_d = \frac{\text{mass in solution}}{\text{volume of water}} = \frac{M_d}{V_w} \quad (6.5)$$

The equilibrium partition coefficient K_d is defined as;

$$K_d = \frac{C_s}{C_d} \quad (6.6)$$

where:

$$\begin{aligned} C_s &= \text{the solid phase concentration (e.g., in soil) [M/M]; and} \\ C_d &= \text{the concentration in solution [M/L}^3\text{].} \end{aligned}$$

The total mass of radionuclides is the sum of the dissolved mass and the mass sorbed in its solid phase, therefore;

$$\begin{aligned} M_T &= M_d + M_s \\ &= C_d V_w + C_s M_{sd} \end{aligned} \quad (6.7)$$

where:

- M_T = total mass of radionuclides [M];
- M_d = mass in solution [M];
- M_s = mass in solid phase [M];
- V_w = volume of solute [L^3]; and
- M_{sd} = mass of sorbent [M].

Substituting Equation 6.7 into Equation 6.6 gives Equation 6.8, which is implemented within RIP.

$$C_{rj} = \frac{M_{rj}}{V_j + M_{sj} K_{drj}} \quad (6.8)$$

where:

- V_j = the user-defined biocell pathway volume [L^3];
- M_{rj} = mass of radionuclide r in pathway j [M];
- M_{sj} = the mass of sorbent (solid phase) in biocell j [M]; and
- K_{drj} = the equilibrium partition coefficient for radionuclide r in biocell j [$L^3 M^{-1}$].

The term $K_{drj} \cdot M_{sj}$ accounts for the fact that not all of the radionuclide mass in a biocell pathway will necessarily be dissolved. Some of it may be sorbed onto solids. For example, suppose we wish to calculate the concentration of radionuclide mass in the water of a pond. The term M_{rj} is the total mass of radionuclides in the pond, including mass that is not in solution. Therefore we need to adapt equation 6.5 (using the term $K_{drj} \cdot M_{sj}$) to only include the dissolved mass in the calculation of concentration.

As discussed in the RIP User's Guide, concentrations in biocell pathways can be specified in terms of mass/volume (e.g., for ponds or streams), or mass/mass (e.g., for soil or biota). In cases where concentrations are specified in mass/mass, the $M_{sj} \cdot K_{drj}$ term would not be applicable and would be specified as 0.

6.2.1.3 Alternative Calculation of Concentrations in Geosphere Pathways

Given the manner in which masses and concentrations are computed within a biocell (as discussed above and in Chapter 4), an alternative way to compute concentrations (and hence doses) for a geosphere pathway is to append a dummy biocell at the end of the pathway. This is done in such a way that the resulting concentration in the biocell is equal to the average concentration in water leaving the preceding geosphere pathway over the time step. The manner in which this is done is described below.

The RIP governing equation for the mass of sorbent in a biocell is given by Equation 6.9.

$$\frac{\partial m}{\partial t} = -mk + q \quad m = 0 \text{ at } t = 0 \quad (6.9)$$

where:

- m = mass in the biocell [M];
- k = turnover rate [1/T]; and
- q = mass flux into the biocell [M/T].

The solution to this equation is;

$$m = \frac{q}{k} (1 - e^{-kt}) \quad (6.10)$$

The mass in Equation 6.10 may be converted into a concentration C (M/L³) by dividing by the volume of the biocell V.

$$C = \frac{q}{kV} (1 - e^{-kt}) \quad (6.11)$$

If the value of k is set by the user such that the term “-kt” is large compared to the size of a time step, then Equation 6.11 reduces to

$$C = \frac{q}{kV} \quad (6.12)$$

Physically this means that the biocell reaches steady state very quickly relative to the length of the time step. If, in addition, the volume of the biocell is set by the user to be equal to the flow rate Q (L³/T) divided by the turnover rate k (1/T), i.e.,

$$V = \frac{Q}{k} \quad (6.13)$$

then the concentration in a biocell becomes,

$$C = \frac{q}{Q} \quad (6.14)$$

The resulting concentration computed in the biocell will be equal to the average concentration in the water leaving the preceding geosphere pathway over the time step.

In summary, to eliminate the difficulties associated with spatial averaging over the pathway the user may add a biocell to the end of the pathway by;

- defining the volume of the biocell (a RIP input) as $V = Q/k$, where Q is the flux leaving the geosphere pathway of interest, and k is the turnover rate for the dummy biocell.

$$\therefore C = \frac{q}{Q}(1 - e^{-kt})$$

- defining the turnover rate (a RIP input) such that e^{-kt} is negligible

$$\therefore C = \frac{q}{Q}$$

6.3 Modeling Health Risk with RIP

RIP assumes a linear relationship between health risk and dose due to exposure to radionuclides. Health risk is assessed in terms of the probability of contracting cancer over a person's lifetime resulting from such an exposure, and can be described by the following equation:

$$LICR_g = D_g \cdot F_{Rg} \quad (6.15)$$

where:

- $LICR_g$ = the annual incremental cancer risk to a member of receptor group g due to the dose received (yr^{-1});
- D_g = annual effective dose equivalent for receptor group g (Sv/yr); and
- F_{Rg} = risk factor for receptor group g (Sv^{-1})

$LICR$ is the annual *incremental* cancer risk associated with a particular dose. The term *incremental* is important because, while there is a natural background cancer incidence rate (approximately 20-25%), our concern is the *increase* above this background rate due to exposure to radionuclides. The fact that a $LICR$ may seem insignificant compared to background levels, and would be epidemiologically imperceptible, is not a concern. Also, the linear $LICR$ equation

is only valid at low risk levels (i.e. below estimated risks of 0.01). If a calculated LICR exceeds this value, the analysis should be carried out in terms of dose alone.

Risk factor values are entered directly as either constant or stochastic values. Risk factor values can be obtained from the literature, but are typically highly uncertain. Therefore, the LICR should generally be reported to only one significant figure. The primary data sources for risk factors are studies of the survivors of the Hiroshima and Nagasaki atomic bombs.

6.4 Dose/Risk Results

As described in detail in the RIP User's Guide, two basic types of dose/risk output can be saved by RIP:

- The peak value (as well as time histories) of the individual risk to each defined receptor;
- The collective risk to all receptors for the entire simulation.

The formula used to calculate this collective population risk is as follows:

$$\text{Total Population Risk} = \sum_{i=1}^N \left[\text{POP}_i * R_i * \left(\sum_{t=1}^T \text{DOSE}_i(t) * \Delta t \right) \right]$$

(6.16)
where:

- POP_i = the population of receptor i;
- R_i = the risk/dose ratio for receptor i [e.g., Sv⁻¹];
- N = the total number of receptors;
- T = the total number of time steps;
- DOSE_i(t) = the dose to receptor i at time t [e.g., Sv/yr]; and
- Δt = the length of the computational time step.

7. THE RIP STRATEGY EVALUATION MODEL

7.1 Basic Concepts

The previous chapters have described in some detail the RIP performance model. However, RIP is also capable of a higher order of modeling, strategy modeling, which is described in this chapter.

The strategy evaluation model was discussed in general terms in Chapters 1 and 2. Additional details are presented in this chapter.

As discussed in Section 2.3, a 'strategy', as used in RIP, refers to a set of activities or elements that are intended to be carried out in order to develop a better understanding of a proposed repository system. The elements of a strategy represent activities such as the following:

- A test or set of tests that are intended to provide additional information about one or more of the parameters that define the performance model. Note that such tests do not always measure the affected RIP parameter directly, and may often measure it indirectly.
- Development of an improved model that will reduce overall model uncertainty. For example, such an activity could consist of developing and making a number of runs of an improved lower-level model of a subsystem. The result might be a modified component model in RIP, or improved RIP parameter precision, or a reduced model-error level.
- Construction of an infrastructure element (e.g. a borehole, or a road), or completion of a required procedural activity such as acquiring a license.

RIP's strategy module allows the user to define strategies, and to evaluate their effectiveness by examining probability distributions of three specific results:

- the *cost of the strategy*
- the *duration of the strategy*
- the *strategy's likely effect on the performance model's predictions.*

Each of these three types of result is evaluated by RIP as a stochastic variable. Thus, RIP provides the user with probability distributions for the overall cost and duration of a strategy. Similarly, RIP provides the user with probability distributions for what the performance-measure distributions may look like after the strategy is carried out. This last item can be a confusing one, because it represents our probabilistic estimate now of what our probabilistic performance estimates will be in the future.

Figures 7-1 and 7-2 show the form of these results. Figure 7-1 shows typical cost and duration probability distributions. Figure 7-2 shows the current probability distribution for system

performance, plus confidence bounds for the distribution after the characterization strategy is executed.

The issue of uncertainty in the cost and duration of a strategy is an important one. While it would be convenient to be able to plan with confidence about the necessary costs and time, in reality neither science, politics, or regulatory bureaucracy is subject to control by the agency attempting to develop the repository. The RIP strategy module contains what is, in effect, a version of the Critical Path Method that incorporates uncertainty.

The general concepts discussed above are best explained by considering an example.

7.1.1 Strategy Evaluation Example

Consider the following example: suppose our current RIP model showed a 90% likelihood of acceptable performance by the repository system. The performance hinged on a single critical issue, which was the possible existence of an undetected fault near to the repository. There was a 10% likelihood that a fault existed, and its existence was necessary and sufficient to cause unacceptable performance of the repository.

A strategy of extensive test drilling was defined for this problem. The drilling would be definitive, so that if the fault existed it would definitely be found. However, the drilling and data evaluation program would be costly and protracted.

The RIP strategy module for this strategy would provide appropriate estimates of the cost and time distributions to carry out the drilling, and would show a likelihood of 90% that subsequently the performance model would show the site was definitely suitable, and a likelihood of 10% that it would be definitely unsuitable.

An alternative program might be proposed, however, which while being significantly quicker and cheaper would be less definitive: it would reduce the uncertainty about the fault by one order of magnitude, so that there would be a 99% confidence in the test result. For this strategy, RIP would show a 90% likelihood that the end product would be a 99% confidence in the site, and a 10% likelihood that the end product would be a 1% confidence in the site.

Depending on the regulatory level of confidence required ('compliance criteria'), and the available cost and time, one of the above two strategies would be preferable. For the second strategy, it might be optimal to plan to reduce the residual 1% uncertainty during a 'performance confirmation' phase subsequent to construction of the repository.

If the real world were as simple as the above example, RIP would not be needed. However, in more realistic situations where there are hundreds or thousands of parameters, which have greater or lesser impact on performance, and where few tests are definitive, the situation can be much more complex. It is here that RIP's strategy module can be valuable, allowing the user to compare and contrast alternative strategies, which may themselves be quite complex, in order to develop an optimal approach.

Results for parameter Cost, 1000 realizations

7-1a Cost

Results for parameter Time, 1000 realizations

7-1b Duration

FIGURES 7-1
**PROBABILISTIC ESTIMATE OF COST
 AND DURATION**
 ARGONNE/MODEL DEVELOPMENT

FIGURE 7-2
EFFECT OF STRATEGY ON PERFORMANCE ASSESSMENT RESULT
ARGONNE/MODEL DEVELOPMENT

7.2 Development of an Activities Database

As discussed in Chapter 1, the RIP strategy module requires the user to construct an activities database. Each entry in the database contains the following information:

- An identifier for the activity.
- A description of the activity.
- The duration of the activity. The duration may be entered as a constant, as a stochastic value, or as a function of other parameters.
- The cost of the activity. The cost may be entered as a constant, as a stochastic value, or as a function of other parameters. In particular, the cost may be a function of the activity's duration.
- A list of any required precedent activities. For each precedent activity, either the start or finish of the current activity can be constrained by the start or finish of the precedent activity, with a user-entered time-lag. For example, an activity could be constrained such that it could not start until three months after its precedent activity finished.
- A list of all performance-model parameters that would be affected by the activity, and the amount of new information about the parameter that would be generated by the activity. The definition of the measure of new information is discussed below in Section 7.3.

7.3 Updating - Simulating the Effect of New Information

The process of updating prior knowledge based on new test results is simulated in RIP, using an algorithm that captures in a simple way what is in fact a very complex process. In RIP, the prior knowledge is expressed in each stochastic parameter's original probability distribution. The prior knowledge input will normally have come from elicitations of one or more experts in the area, based on reviews of experimental data and available modeling results.

RIP's algorithm for updating is based on Bayesian updating of a parameter. Bayes' theorem states that, for some particular value x of parameter X :

$$p'(x) = \frac{p(x) (p(x_i|x))}{p(x_i)} \quad (7.1)$$

where:

$p'(x)$ =	updated probability of x ;
$p(x)$ =	current probability of x ;
$p(x_i x)$ =	probability of test result x_i given that x was the true value; and
$p(x_i)$ =	current probability of test result.

The updated distribution is often referred to as the 'posterior' distribution. Note that the test result does not have to be a measurement of X itself: the test need only measure some value that is affected by the value of X . For example, the parameter X might be the annual precipitation at a site, whereas the test might measure the moisture content in the soil. A considerable amount of additional information, plus some modeling, would be needed to derive the relationship between soil moisture content and precipitation.

Figure 7-3 shows graphically the process that RIP uses to simulate updating. It is essentially a two-step approach to updating: 1) first RIP simulates (by Monte Carlo sampling) the value of x implied by the test result, x_i ; and 2) then it computes an updated ('posterior') distribution for X .

The user is required to define a term called the *test standard deviation*, which represents the level of uncertainty in the test-generated estimate x_i . The test standard deviation is input in a normalized form as a multiple of the prior standard deviation of X . For example, if the prior probability distribution of a rock property was based on 16 samples, and a test was planned that would evaluate 9 more samples, the test standard deviation would be 1.33 of the prior (because the standard deviation of a sample mean varies inversely with the square root of the number of samples). If the new test was to evaluate 100 samples, the test standard deviation would be 0.4 of the prior's.

Hence, a test standard deviation greater than one implies that the test provided a smaller amount of information than the prior, a test standard deviation equal to one implies that the test provided an amount of information equal to that currently supplied by the prior, and a test standard deviation of less than one implies that the test provided a larger amount of information than the prior. A test standard deviation of 0 implies that the test was definitive: there would be no remaining uncertainty after the test.

RIP generates a value for x_i by randomly realizing the 'true' value of X (based on the prior distribution), and then randomly realizing the test result x_i based on the true value and the test standard deviation. The process of Bayesian updating of the prior distribution for X is then carried out.

The probability distribution of x_i uses a normal distribution. The updating process also uses a normal distribution, in order to compute the 'probability of the test result if x was the true value'. This distribution is evaluated for a series of values x_i , using logic similar to that described above, and is used to evaluate the likelihood of having seen x_i if the real result was x_i .

1. Prior distribution of x

2. Realize 'true' value t
3. Construct distribution of test result based on "true" value and test standard deviation
4. Realize test result x_t

5. Bayesian update:
 $p'(x) \propto p(x) p(x_t|x)$

6. Normalize the posterior p'

FIGURE 7-3
 SIMULATING EFFECT OF NEW INFORMATION
 ARGONNE/MODEL DEVELOPMENT

Regardless of the form of the prior distribution of X , the output is a 10-point 'cdf' cumulative distribution. The range of the output distribution is the same as the prior, and the internal points are arranged so as to best represent the true shape of the distribution's curve.

In order to gain computational efficiency, RIP short-cuts calculating the denominator in Bayes' theorem by normalizing the posterior distribution to have a total probability of unity. This is a valid approach that does not affect the result.

7.4 Strategy Evaluation Results

7.4.1 Strategy Cost and Time Distributions

Probability distributions for cost and elapsed time can be displayed for any stage of the strategy. These distributions are developed by Monte Carlo realizations of the entire strategy, using the methods described elsewhere in this report. These displays are available from the RIP module in which the user defines the strategy activities.

7.4.2 Effect of a Strategy on a Parameter

Within the parameter-editing portion of RIP it is possible to evaluate the sensitivity of any stochastic parameter or function of stochastic parameters to the selected strategy. The result is a display of probability distributions of different quantiles (eg, the 0.9 exceedance level) for the parameter subsequent to carrying out the strategy.

The results are developed by repeatedly executing the strategy and doing Bayesian updates of all the affected parameters from their prior probability distributions. The probability distribution of the parameter being studied is evaluated using the updated distributions, and the different quantiles (0.01, 0.1, 0.5, 0.9, 0.99) are evaluated and saved. After a number of repetitions of this process, it is possible to develop the distributions of each quantile subsequent to carrying out the strategy.

7.4.3 Effect of a Strategy on Performance Assessment Results

Within the RIP post-processing module, the user can evaluate the effect of the proposed strategy on any of the performance results calculated by RIP. This evaluation is made not by re-running the back end, but by re-evaluating the relative likelihood of each previously-evaluated realization. In this way it is possible to rapidly evaluate alternative strategies without the time-consuming necessity of re-running the back end. The result of such an evaluation has a form similar to that shown in Figure 7-2.

It is important to note that the algorithm used to carry out the strategy evaluations is only valid if the reduction in uncertainty in a parameter is relatively small (less than an order of magnitude). For large reductions in uncertainty, the results could be erroneous. This is because, as stated above, RIP does not resample the updated distributions; it simply adjusts the

weights of the original sampled values appropriately. If the reduction in uncertainty for a parameter was quite large, the original sampled values may not include enough values that fall within the range of the updated distributions. This would cause poor representation of the updated distributions and possibly erroneous results.

7.5 Summary of the Strategy Evaluation Model

The strategy portion of RIP provides the second cornerstone of the Golder approach by quantitatively integrating the performance assessment model with the characterization activities. The strategy model is essentially a decision analysis shell around the performance assessment model that allows the user to evaluate alternative site characterization strategies.

For any user-specified characterization strategy, RIP provides three outputs by which alternative strategies can be ranked and compared:

- a probabilistic estimate of cost;
- a probabilistic estimate of duration; and
- a probabilistic evaluation of the predicted site performance resulting from implementation of the strategy.

Computation of the first two outputs is straightforward, and consists of integrating within a Monte Carlo framework the cost and duration estimates for the individual activities, taking into account any precedence requirements. The third output relies on subjective assessments by experts of the extent to which model parameter uncertainty will be reduced by a particular activity. Given these assessments, along with the current state of knowledge, RIP uses a Bayesian computational algorithm to simulate how probability distributions representing parameter uncertainty will change as a result of a particular characterization strategy, and develops a probabilistic evaluation of the anticipated repository performance.

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APPENDIX A

METHODS FOR DEVELOPING DEFENSIBLE SUBJECTIVE PROBABILITY ASSESSMENTS

METHODS FOR DEVELOPING DEFENSIBLE SUBJECTIVE PROBABILITY ASSESSMENTS

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ABSTRACT

Typically, some degree of uncertainty exists in the scenarios and value of parameters at any site (e.g., due to insufficient data, natural spatial variability, or possible changes with time). Often, this uncertainty must be quantified (e.g., in terms of probability distributions that express the relative likelihood of any value). Because of inevitable data base deficiencies, those probability distributions must be based to some degree on subjective assessments, reflecting personal opinions and judgment, consistent with all available information (site-specific and generic) and recognizing the entire range of possible values. Subjectively derived probability distributions can represent the opinions of individuals or of groups. There are problems associated with either, which, if uncorrected, render the results suspect and difficult to defend. Various techniques have been developed to conduct subjective probability assessments with varying effort and success in mitigating such problems. Thus, the appropriate technique is that which provides the desired level of defensibility at least cost.

INTRODUCTION

Various scenarios can occur at a site, and the associated parameters are often complex, varying spatially and, in some cases, with time, as a function of scale and possibly other factors. The scenarios and values of parameters must often be estimated (e.g., for analysis and design). However, data bases regarding these scenarios/parameters, in many cases, will contain a small number of samples and inexact representation of the true conditions, because of the cost involved in gathering representative data. Scenarios/parameter values cannot be determined accurately in such cases where the data base is statistically insufficient. Instead, the scenarios/parameter values must be estimated based on whatever information is available, including generic as well as site-specific data. Those estimates, depending on their application, may represent conservative assumptions (e.g., to demonstrate compliance with some criteria) or best guesses (e.g., to predict actual performance of alternatives as input to decision making). Such estimates must necessarily incorporate interpretations and judgments regarding the data base, which are subjective and in many cases non-unique, and thus may be open to controversy. Controversy can significantly delay a project and cause unnecessary expense, especially if an ultra-conservative assumption results. Hence, the objective is to cost effectively produce appropriately defensible estimates of scenarios/parameter values where significant uncertainty exists and must be subjectively assessed.

Many examples of such uncertainty analyses exist¹. This paper is derived from a detailed manual developed by the author specifically for conducting subjective probability assessments².

UNCERTAINTY/PROBABILITY CONCEPTS

Variables can represent 1) the state at a particular place and time, or 2) where the state may vary spatially and/or temporally, a group statistic (e.g., mean or variance of the population). The variables, in either case, would have a unique value. Moreover, such variables may be "continuous" (i.e., each may have an infinite number of possible states) or may be "discrete" (i.e., each may have a finite number of possible states).

Often, the state of a variable has not been directly and accurately observed, and there will generally be some uncertainty as to what the state of that variable actually is, was, or will be. The possible sources of this uncertainty can be summarized as follows²:

- **Statistically insufficient data:** In direct observations of a variable state, measurement errors (random or systematic) and accuracy limitations may exist. Where the state has not been directly observed, it must be inferred (e.g., interpolated, extrapolated, or analytically derived) from other information. In analytically deriving a variable state from other site- and time-specific measurements, there may be imperfect understanding regarding the processes involved and approximations and simplifications in the analytical procedure. The applicability of indirect observations in the inference of the variable state must be considered. In assessing group statistics, there may not be enough data to be statistically significant or the data may not accurately represent the population (i.e., biased sampling).
- **Natural spatial and/or temporal variability:** The variable state may vary spatially or temporally (i.e., change with time) or both. For example, the space may not be homogeneous and uniform, and may instead have heterogeneities, or the variable state may be affected by future events that cannot be predicted with certainty. In interpolating or extrapolating from observations (direct or indirect) elsewhere and/or at other times, this spatial or temporal variability and the effects of heterogeneities and of events and processes (both past and future) must be considered.

The uncertainty in the actual state of a variable can be quantitatively expressed in various related ways (e.g., ranges, accuracy measures, confidence levels, or probability distributions)³. As illustrated in Figure 1, probability distributions can be defined for:

- **Discrete variables** (Figure 1a), in terms of a probability mass function (pmf), which expresses the probability of each possible variable state.
- **Continuous variables** (Figure 1b), in terms of:

- probability density function (pdf), which expresses the relative likelihood of each possible variable state; and/or
- cumulative distribution function (cdf), which expresses the probability that the variable state will be less than or equal to each possible variable state.
- **Group statistics** (Figure 1c), in terms of pdfs and/or cdfs for:
 - mean (μ_x), first moment about zero;
 - variance (σ_x^2), second moment about the mean;
 - standard deviation (σ_x), square root of the variance; and/or
 - other higher moments of a distribution.
- **Multiple variables** (Figure 1d), in terms of:
 - joint pmf/pdf, which expresses the probability or relative likelihood of each possible combination of discrete or continuous variable states actually occurring;
 - marginal pmf/pdf, which expresses the probability or relative likelihood of each possible state of one variable actually occurring, regardless of the state of the other variable;
 - conditional pmf/pdf, which expresses the probability or relative likelihood of each possible state of one variable actually occurring given the state of another variable; and/or
 - covariance function/correlation coefficient, which expresses the relationship of the state of one variable to the state of another variable (including spatial and temporal correlation).

INDIVIDUAL PROBABILITY ASSESSMENT TECHNIQUES

The potential problems associated with a single individual subjectively developing probability assessments include the following²:

- **Poor quantification of uncertainty:** The assessor might not express uncertainty in a self-consistent or proper fashion. It has been shown⁴ that people not trained in probabilistic analysis typically have problems in accurately quantifying their uncertainty. For example, if someone expresses a 90% probability or level of confidence that something will happen, it should happen nine out of 10 times on the average under similar circumstances. However, typically when verified, it has been shown that the event happens much less than nine (more like five) out of 10 times.
- **Poor problem definition:** The parameter for which the value is to be assessed might have been ambiguously defined so that the basis of the assessment might not be correct. For example, in assessing the value for hydraulic conductivity with respect to groundwater flow through the site, the scale (large-scale averages versus small-scale laboratory values) might not have been specified.

- **Unspecified assumptions:** The assessor might not specify (or even be aware of) the assumptions which underlie his/her assessment so that the conditional nature of the assessment might not be apparent. For example, the assessor may have assumed porous flow through the rock mass rather than considering flow through intersecting fractures in assessing the value for average hydraulic conductivity with respect to groundwater flow through the site.
- **Uncorrected biases:** The assessor might not specify (or even be aware of) biases which underlie his/her assessment, so that the assessment does not accurately reflect the assessor's knowledge. Biases fall within various categories:
 - **"Motivational",** where the assessor's statements and conscious beliefs are inconsistent. Motivational biases, in turn, can be categorized as follows:
 - * **"Management" bias** refers to the assessor's possible view of an uncertain variable (e.g., as an objective rather than an uncertainty). For example, if the objective is to achieve a low groundwater flow through the site, then the average hydraulic conductivity may be understated.
 - * **"Expert" bias** refers to a possible reaction that the assessor may have to being considered as an expert. The assessor may feel that experts are expected to be certain of things. This bias tends to promote central bias (i.e., a tendency for the assessor to understate uncertainty). For example, the assessor may understate the range in the average hydraulic conductivity of a specific site.
 - * **"Conflict" bias** refers to a reward structure that might encourage the assessor to bias the estimates high or low. For example, an unethical assessor might understate the value of a significant parameter (e.g., average hydraulic conductivity), if it was personally beneficial (e.g., to make a project appear feasible).
 - * **"Conservative" bias** refers to the assessor's desire to err on the safe side. For example, if an event has an adverse impact, then the assessor may want to avoid underestimating the probability of that event (e.g., by consciously overstating its probability), thereby bounding the assessment rather than truthfully estimating it.
 - **"Cognitive",** in which the assessor's conscious beliefs do not reflect the available information. Cognitive biases, in turn, can be categorized as follows:
 - * **"Anchoring"** refers to the tendency of individuals to produce estimates by starting with an initial value (suggested perhaps by the formulation of the problem) and then adjusting the initial value to yield the final answer. The adjustment is typically insufficient. For

example, the assessor might estimate the most likely value first and then the range in possible values, where this estimated range would probably be larger if assessed first.

- * **"Availability"** (or incompleteness) bias refers to the fact that if it is easy to recall instances of an event's occurrence (e.g., the event had some personal significance to the subject), then that event tends to be incorrectly assigned a higher probability. For example, if the assessor had been involved previously with a high groundwater flows, then the resulting assessment of the average hydraulic conductivity would tend to be higher than without this experience.
- * **"Base rate"** bias (or lack of moderation, law of small numbers) refers to the tendency of the assessor to focus only on specific information. Empirical evidence shows that assessors often tend to attach less importance to general information. For example, if the specific information is some recent data (e.g., the results of recent field tests), then the importance of that information might be overrated in the assessor's mind.
- * **"Coherence and conjunctive distortions"** refers to the tendency of an assessor to not properly account for and combine all of the components of a problem. For example, in assessing groundwater flow where various parameters (e.g., average hydraulic conductivity, gradient) must all be within specific bounds for the flow to be acceptable, people seem especially prone to overestimating the probability that the flow will be acceptable.
- * **"Representativeness"** refers to the tendency of an assessor to treat all information equally, even though it may not be statistically representative. For example, intact rock (with low hydraulic conductivity) may be more easily sampled than highly fractured rock (with high hydraulic conductivity) so that there is a larger percentage of low hydraulic conductivities in the laboratory data base than there is in reality. If this sampling bias was not recognized, the average hydraulic conductivity might be underestimated.
- * **"Overconfidence"** refers to the tendency of an assessor to underestimate the uncertainty about the value of a parameter. For example, the assessor might not recognize and properly account for other possible values of the parameter.
- * **Imprecision:** The assessor may be indifferent over a specific range of values, so that there is some "fuzziness" in the assessments. For example, an assessment of 20-30% probability that something will happen should be able to be refined further with additional consideration.

- * **Lack of credibility:** If the assessor cannot be considered an expert in the technical field, the assessment (regardless of the other limitations) may lack credibility. Such an assessment would not be defensible to other experts or, often more importantly, to the public. For example, a recent graduate engineer with little experience should not be making critical assessments alone.

As summarized in Table 1, the techniques available for eliminating or mitigating the potential problems associated with developing individual subjective probability assessments, include the following²:

- **Self-assessment:** The simplest approach to developing an individual subjective probability assessment is "self-assessment"^{5,6}, where the analyst interprets the available information and quantifies an assessment of the likely value and its uncertainty. The rationale behind the assessment should be well-documented, including a description of the available information and an evaluation of that information, to enhance defensibility of such subjective probability assessments. Although attractive because of its obvious simplicity, this method has significant limitations:
 - poor quantification of uncertainty;
 - uncorrected biases and/or unspecified assumptions, possibly in spite of documentation;
 - imprecision; and
 - lack of credibility, if the analyst cannot be considered an expert in the technical field.
- **Informal solicitation of expert opinion:** One of the most common methods of developing an individual subjective probability assessment consists of "informal solicitation of expert opinion"^{7,8}, where the analyst asks an "expert" to interpret the available information and quantify an assessment of the likely scenario or value of a parameter, and its uncertainty. The defensibility of such assessments is increased over self-assessment techniques due primarily to the increased credibility of the expert involved. As for self-assessment, the expert's rationale for the assessment should be well-documented, including a description of the information available to the expert as well as the expert's evaluation of that information, to further enhance defensibility of subjective assessments. Although generally an improvement over self-assessment techniques, due to increased credibility, informal solicitation of expert opinion has similar significant limitations, as well as increased cost and potentially poor problem definition.
- **Calibrated assessment:** A systematic approach to developing an individual subjective probability assessment is through the use of "calibrated assessments"⁹⁻¹¹, where the assessor's biases are identified and calibrated, and the

assessments are adjusted to correct for such biases. Hence, two sets of assessments are required:

- the assessor's assessment (e.g., through the informal solicitation of expert opinion); and
- an assessment of the assessor's biases.

The assessment of the assessor's biases can be done either: subjectively by peers (i.e., in the same way as other subjective assessments), or objectively through a set of experiments or questionnaires. The objective approach typically consists of asking the assessor a series of questions for which the true answer is available but unknown to the assessor. For example, the assessor's identified biases can be corrected in the following way:

1. the assessor may be given a set of relevant data which does not include the direct measurement of the parameter of interest even though such a measurement exists;
2. the assessor estimates the parameter value based on the available data;
3. the assessor's estimate is compared with the true value, as given by the measurement; and
4. a correction or calibration factor is determined for the assessor, which when applied to the assessor's estimate results in the true value.

Although, a general improvement over self-assessment or informal solicitation of expert opinion techniques, due to the mitigation of some biases, calibrated assessments entail similar significant limitations (even after calibration) as well as increased costs and inherent difficulties in objectively determining calibration factors for many of the scenarios/parameters of interest, since direct measurements might never be available for verification and the calibration factor may not be constant in any case.

- **Probability encoding:** The most systematic and defensible approach to developing individual subjective probability assessments, but also the most expensive, is "probability encoding"^{1,12-15}. In probability encoding, analysts trained in probability theory elicit in a proper and self-consistent manner a technical expert's assessment of the pdf of scenarios or a parameter value, which expresses that expert's uncertainty in the value in quantified terms. This is done in a formalized way² in five stages:
 1. motivating;
 2. structuring;

3. conditioning;
4. encoding; and
5. verifying.

During this process the analyst attempts to:

- train the subject to properly quantify uncertainty;
- identify and minimize the subject's bias tendencies;
- define (and document) the item to be assessed in an unambiguous manner;
- elicit and document the subject's rationale, including the available information, for assessment;
- elicit (directly or indirectly) and document the subject's quantitative assessment of uncertainty and check for self-consistency; and
- verify the assessment with the subject, repeating the process if necessary.

As illustrated by the example given in Figure 2, the subject's quantitative assessment of uncertainty can be elicited indirectly by determining the probability of various states through:

- comparison with familiar reference events (e.g., poker hands); or
- choosing between two lotteries (e.g., probability wheel or intervals, Figure 2a and b), until indifference is achieved.

A cdf can then be defined, consistent with the various assessments (Figure 2c). Although a general improvement over other available methods, due to mitigation of most of the potential problems, some imprecision may remain and probability encoding is relatively costly because it is labor intensive.

CONSENSUS PROBABILITY ASSESSMENT TECHNIQUES

Differences may exist in the assessment of individuals comprising a group, which may arise from a number of sources, including²:

- **Disagreement on the assumptions or definitions that underlie assessments:** Individual assessments are based on specific assumptions and definitions. If these assumptions and/or definitions differ between individuals, then the individual assessments may differ. For example, one individual may have ruled out a specific case that another individual assumes likely, or one individual may

have defined the parameter of interest at a different scale than another individual.

- **Failure to overcome assessment errors and biases:** In conducting the individual assessments, a key objective is to eliminate anchoring, availability, overconfidence, and other common distortions. Training individuals and allowing them to practice making probability judgments prior to the individual assessment help to overcome biases, but such errors may persist. For example, overconfidence may have been mitigated to a large extent in one individual's assessment but not in another's, so that although the means of their probability distributions may be similar the variances may be significantly different.
- **Judgments based on differing information sources:** Both specific data and general knowledge are relevant to the encoding process. Such knowledge varies even among highly specialized experts. Specific information may vary in quantity and quality, while general information may vary due to differences in training and experience. For example, one individual may have based an assessment on a specific data set in conjunction with his/her personal experience, whereas another individual may have used a different specific data set in conjunction with different personal experience.
- **Disagreement on how to interpret available information:** The available information must be interpreted by the individuals. In this interpretation, individuals may disagree, for example, on the methods used to obtain data, the relevance of such data to the quantity being assessed, or on the appropriateness of a particular theory or model. For example, individuals may disagree on how to interpret well stem tests and their validity to assessing large-scale hydraulic conductivities at a site with respect to groundwater flow.
- **Different opinions or beliefs about the quantity of concern:** Even after agreeing on the basis for the assessment, the information available, and how to interpret this information, individuals may still have a difference of opinion. For example, individuals may arrive at different pdf's for average hydraulic conductivity, even after agreeing on all the preliminary aspects.

It is typically desirable to attempt to resolve these differences of opinion, with the following outcomes possible:

- **Convergence:** A single assessment is determined that expresses the common belief of all individuals in the group, as expressly agreed to by the group members.
- **Consensus:** A single assessment is determined, although the assessment may not reflect the beliefs of each individual; the consensus assessment may be derived from the individual assessments without the express agreement of the individuals (forced) or it may be expressly agreed to by the group for a particular purpose (agreed).

- **Disagreement** Multiple assessments are determined where convergence or consensus on a single assessment is not possible (e.g., owing to major differences of opinion).

In general, convergence is generally most desirable, as it is most defensible, but may be difficult to achieve. Agreed consensus, i.e., with the concurrence of the group, is slightly less defensible but also less difficult to achieve. Forced consensus, without concurrence of the group, may be difficult to defend but is very simple. Disagreement may be difficult to use, as it is non-unique, but is defensible.

Techniques available for resolving differences of opinion amongst a group of individual assessors can be categorized in terms of "mechanical aggregation" and "behavioral procedures":

- **Mechanical aggregation** of individual assessments is a relatively simple approach to achieving at least forced consensus, and involves applying a mathematical formula or procedure to combine the various individual probability distributions^{16,17}. If the individuals in the group agree to the resulting distribution, then agreed consensus (and possibly convergence) can be achieved. In general, mechanical aggregation techniques are most useful when the means, rather than the variances, of the individual probability distributions differ. Also, mechanical aggregation techniques can be used when a single distribution is required, but the scenario/parameter in question is not significant enough to warrant large amounts of effort to achieve convergence or agreed consensus.

The various forms of mechanical aggregation include the following²:

- **Averaging**, which is the simplest mechanical aggregation technique, involves simply averaging the individuals' probabilities for each possible value. Several empirical studies^{18,19} have shown that averaged probabilities are often superior to individual assessments. As an example, if one individual assessed an 80% probability of the average large-scale hydraulic conductivity (log) being less than -3.5 and the other individual in the group assessed a 60% probability, then the group average would be a 70% probability.
- **Group statistics**, which is a somewhat more rigorous treatment, involves determining the group's distribution of opinions regarding the probability for each value, thereby developing a "fuzzy" assessment or an assessment which corresponds to a given level of conservatism for the group. More complete statistical methods are available that incorporate dependence among variables and experts⁹ and least squares or partitioning methods²⁰. As an example, the statistics of the group members' opinions of the probability of the average large-scale hydraulic conductivity (log) being less than -3.5 could be determined and used.
- **Weighting methods**, which are elaborations on either averaging or group statistics, involve the weighting of individual assessments by an external

procedure to incorporate biases or differing levels of expertise among the individual assessors, similar to individual calibrated assessments. There are essentially two weighting procedures:

- * "calibration exercise", in which the natural biases and tendencies of the individual assessors are evaluated and mitigated through 1) the administration of a series of general questions to determine each assessor's ability to make correct assessments, and 2) the determination and application of weighting factors for each assessor to reflect that assessor's ability (relative to the other assessors) to make correct assessments; and
 - * "peer ratings", in which each of the individual assessor's relative ability to make correct assessments is assessed subjectively by peers, although such a subjective assessment may itself introduce additional biases.
- **Behavioral procedures** can be used to attempt to develop convergence or at least agreed consensus, and involve interaction among the individuals in the group, which allows for the explicit identification and resolution of differences of opinion. Although there is evidence that such interaction results in better assessments^{21,22} and that the results are generally more defensible, because the group agrees on a given distribution, behavioral procedures tend to entail significantly more effort, because the various individual assessors must be involved. Such behavioral procedures are necessary when at least agreed consensus (or disagreement) is required (i.e., for significant parameters), and are especially useful when the differences between the individual assessments are large.

As summarized in Table 1, the various forms of behavioral procedures include the following²:

- **Open forum** is a very informal means of achieving consensus and does not require prior individual assessments. The group attempts to achieve convergence or agreed consensus by open discussion of whatever each individual deems important to resolving the problem. A major limitation of this method is that the result can be distorted by the dynamics of the group, such as domination by an individual because of status or personality²³. For example, the persuasiveness of a vocal individual or the desire of some individuals to avoid dissension may distort the results. Other potential limitations to this method are the same as for the development of individual assessments through the informal solicitation of expert opinion, i.e., poor quantification of uncertainty, uncorrected biases, unspecified assumptions, and poor problem definition. The method is also limited by the credibility of the group members.

- **Delphi panel** is a systematic and iterative approach to achieving consensus, and has been shown to generally produce results which are reasonably reproducible across independent groups^{22,24-27}. Each individual in a well-defined group is provided with the same set of background information, and is asked to conduct and document (in writing) a self-assessment. These assessments are then provided anonymously to each of the other assessors, who are encouraged to adjust their assessments in light of their peers' assessments. Typically, the individual assessments tend to converge. Such iterations are continued until either consensus is achieved or the results stabilize otherwise (i.e., disagreement). Because the Delphi technique maintains anonymity and independence of thought through physical separation of the panelists, it precludes the possibility that any one member of the panel may unduly influence the others due to actual or perceived personality dominance. Otherwise, it tends to have limitations similar to those for open forum.
- **Group probability encoding** is a formal process in which a single probability distribution is assessed directly from a group of individuals, such as for the development of individual assessments by probability encoding¹. However, this requires the group to reach agreement on each question posed during the encoding process, which would be a difficult and tiresome procedure. As for the open forum, face-to-face interaction among participants can create destructive pressures within the group and distort the results.
- **Formal group evaluation** is a formal process of resolving differences between previously developed individual assessments¹. This process is similar to probability encoding in that it is a joint undertaking between a trained analyst and, in this case, a group that has completed individual assessments. It consists of six steps:
 - 1) motivating;
 - 2) identifying differences in the individual assessments;
 - 3) discussing the basis for each individual assessment;
 - 4) discussing information sources and interpretations;
 - 5) re-encoding (if warranted); and
 - 6) reconciling differences).

In this process the analyst fulfills an essential role in questioning and probing the group, helping them to understand the differences, and guiding them through the resolution process, often conducting group re-assessments. This sharing of knowledge tends to produce a commonality (i.e., in definitions, assumptions, information bases, and interpretations) that is a key step in reducing the differences between individual assessments. As for open forums, face-to-face interaction among participants can create destructive pressures within the group and distort

the results. However, the analyst can be alert to such pressures and mitigate their effects to a large extent.

RECOMMENDED PROCEDURES

As summarized in Figure 3, the recommended procedure for selecting the appropriate subjective probability assessment technique consists of the following steps²:

1. Prior to conducting subjective probability assessments:
 - develop the model(s) for the system of interest, e.g., a model would be needed to determine groundwater flow;
 - conduct sensitivity studies to determine the relative significance of each of the various scenarios and model parameters, e.g., sensitivity studies on the model might show that groundwater flow is very sensitive to the average large-scale hydraulic conductivity at the site; and
 - obtain the available data regarding the various scenarios/parameters, where the relative significance of each scenario/parameter will determine the appropriate level of effort in gathering data, e.g., the data on hydraulic conductivity might be limited to inference from measured physical properties, as well as generic information.
2. Each scenario/parameter to be assessed, on the basis of the model, must be defined unambiguously, e.g., considering temporal and spatial variability, as well as conditional factors (such as scale). Also, it may be useful to decompose a scenario or parameter into more elemental variables for assessment. For example, hydraulic conductivity might be defined as being large scale (i.e., averaged over 10's of meters), recognizing that the value may vary spatially within one geologic unit, as well as within the time frame of interest (i.e., 1000's of years). Hydraulic conductivity could be defined separately for the rock mass (e.g., for equivalent porous flow analyses) or for fractures (e.g., for fracture flow analyses). Hydraulic conductivity could be decomposed into permeability and viscosity.
3. The appropriate level of assessment must be determined on the basis of relative significance of each scenario/parameter to be assessed (from sensitivity studies). For example, if a parameter is relatively insignificant (e.g., density), a low level assessment (with corresponding low costs and low defensibility) would be appropriate. However, if a parameter is relatively significant (e.g., hydraulic conductivity), a high level assessment (with corresponding high costs and high defensibility) would be appropriate. For cost-efficiency, high level assessments should only be used for the most significant scenarios/parameters where high defensibility is required, thus justifying their high costs.

4. The most cost-effective assessment technique is chosen (Figure 3) on the basis of the necessary level of assessment and, in conjunction with the data base, implemented for each scenario//parameter (e.g., using specific procedures²).

SUMMARY AND CONCLUSIONS

Subjective probability assessments must often be made (e.g., to accurately predict performance and/or to make decisions among alternatives) wherever the data are not statistically sufficient to make objective assessments. Such subjective probability assessments must be defensible enough to adequately resolve potential controversies. The required defensibility of such assessments is proportional to the significance of each parameter being assessed (e.g., as determined by sensitivity studies).

Potential problems have been identified that are associated with developing individual subjective probability assessments and with developing consensus subjective probability assessments amongst a group that, if uncorrected, can affect defensibility of the results. The available techniques for addressing these potential problems, with varying success and effort, have been presented. Procedures for cost-effectively conducting appropriately defensible subjective probability assessments have been developed.

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TECHNIQUE	POTENTIAL PROBLEMS						
	Poor Quantification of Uncertainty	Poor Problem Definition	Uncorrected Biases/ Unspecified Assumptions	Imprecision	Lack of Credibility	Group Dynamics	Expense
INDIVIDUAL							
Self Assessment	●	○	●	●	●	NA	○
Informal Solicitation of Expert Opinion	●	●	●	●	◐	NA	◐
Calibrated Assessment	◐	●	◐	●	◐	NA	◐
Probability Encoding	○	○	○	◐	◐	NA	◐
GROUP (BEHAVIORAL)							
Open Forum	●	◐	●	●	◐	●	●
Delphi Panel	●	◐	◐	●	◐	○	●
Group Probability Encoding	○	○	○	◐	◐	◐	●
Formal Group Evaluation	○	○	○	◐	◐	◐	●
<p>● Technique does not significantly mitigate potential problem</p> <p>◐ Technique partially mitigates potential problem</p> <p>○ Technique effectively mitigates potential problem</p>							

Table A-1. Evaluation of Subjective Assessment Techniques

a) Discrete Variable (e.g., a scenario)

b) Continuous Variable (e.g., a parameter with a unique value)

c) Group Statistics (e.g., a parameter with a population of values)

d) Joint, Marginal, and Conditional pdf's

Figure A-1. Probability Distributions

a) Probability Wheel

"Which would you rather pick?"
(Change size of black area until indifferent)

vs.

"The average large-scale hydraulic conductivity (log) at a site will be less than -3.1."

b) Interval Technique

"Which interval would you rather pick?" (Change threshold value until indifferent)

"The average large-scale hydraulic conductivity (log) at a site will be less than -3.5."

vs.

"The average large-scale hydraulic conductivity (log) at a site will be greater than -3.5."

c) Cumulative Distribution Function

Figure A-2. Probability Encoding Examples

Figure A-3. Procedure for Selecting Technique

APPENDIX B

DISCUSSION OF SCENARIO AND SIMULATION APPROACHES TO PERFORMANCE ASSESSMENT MODELING

The reader will note that the RIP model does not directly incorporate the concept of a 'scenario'. RIP treats all possible states of the repository system, and all possible future states of nature, as alternative realizations of a single 'universal' scenario. This approach differs from that taken by many other organizations, and is compared to other approaches in the following discussion.

There is a general consensus within the international community involved with long-term disposal of radioactive wastes that safety-assessment should be founded on a "scenario-consequence" modeling approach (NEA,1991). That is, a number of scenarios should be identified which represent possible futures for the repository system, and the likelihood and consequences of each scenario should be evaluated. The overall safety of the repository system would then be evaluated by combining the scenario consequences appropriately weighted by their likelihoods.

However, the term 'scenario' is used in a number of different ways, and there has been some confusion and debate as to the 'proper' definition of a scenario. There appear to be at least five points at issue:

- 1) Should a scenario just define the behavior of the external environment as it affects the repository, or should a scenario define the condition of both the external environment and the repository system itself?
- 2) Should a scenario be developed for each possible significantly different behavior of the system, or should 'archetype' scenarios be developed which each are considered to be representative of a set of similar scenarios? (For example, a 'drilling' scenario could be developed which would be considered to be representative of (or a worst-case of) all drilling intrusion cases).
- 3) Should scenarios be used to refer only to future changes which might affect the repository system, or should they also incorporate possible different behaviors due to uncertainty in the as-built system? (For example, there might be some possibility of an undetected fault at a site: should that be a scenario?)
- 4) Should scenarios or scenario-classes be defined externally to the modeling system, or generated within the stochastic model(s) itself?
- 5) Where there is an unresolved dispute as to which one of several alternative conceptual models is the most appropriate, is it valid to assign likelihoods to each model, and weigh the models into the combined probability distribution of system performance?

For mathematical validity, it is essential that whatever definitions are used, the set of scenarios must be comprehensive (i.e. represent all significant behaviors) and mutually exclusive (i.e. do not overlap).

The choice of how to interpret the above points at issue is essentially one of convenience: for each interpretation of what a 'scenario' is, it is possible to develop a completely valid system model. (It is also quite easy to develop a less than completely valid model, if sufficient care is

not taken). The issues of convenience relate to such factors as ease of defining the necessary scenarios, computational expedience and efficiency, ease of interpreting the output of the models, ease of looking at 'what if' questions, etc.

Guzowski (1990) provides a synopsis of different approaches to scenario development that have been taken, and summarizes the approach used for the Waste Isolation Pilot Plant (WIPP). NRC (1990) describes an approach quite similar to that used at WIPP. The Yucca Mountain Site Characterization Plan (DOE, 1988) proposes a quite different approach, as set out in the following table.

TABLE B.1

Issue	WIPP	NRC	DOE-SCP	RIP
External/Internal Processes?	Both*	External only	Both	Both
Archetype Scenarios?	No*	?	No	No
Future Changes Only?	No	Yes	No	No
Scenarios Built-In to the Model?	No	No	No?	Yes ¹
Apply Probabilities to Alternate Conceptual Models?	No	No	?	1

Note: the above table represents the authors' interpretation of the cited references.

* no final decision made yet

? means not discussed in the reference

1 a user option in RIP

There is a general uniformity by the authors of all of the above references, in that the particular method they selected, while perhaps imperfect, is seen as avoiding the pitfalls that alternative methods will fall into. The authors of RIP feel no differently. The approach taken in RIP, direct simulation, has been suggested to have several drawbacks. The following notes address these perceived drawbacks, and the ways in which RIP attempts to minimize them.

- Combining 'internal' with 'external' processes and events makes it difficult for the regulators and the public to directly address 'what if' questions.* This is a valid issue, as simply producing a CCDF probability distribution from a 'black box' model will not provide the degree of understanding of the overall repository system's behavior that will be needed to produce confidence. RIP's approach, however, allows this issue to be addressed in two different ways:

 - 1) The defining probabilities can be altered by the user so that a particular event always occurs. The resulting system behavior then represents a scenario model, and can be studied and interpreted appropriately.

- 2) When a massive RIP analysis, involving possibly thousands of simulations is performed, the individual system simulations are not discarded. The inputs to and the response of the system for each realization are retained for further analysis. The RIP user can selectively display subsets of the results in order to further evaluate the system's performance. For example, the user could select and review the results of all simulations involving volcanic events, or all simulations involving increased precipitation. This capability should provide a very powerful ability to develop an understanding of the system's behavior.
- *Excessive numbers of simulations will be required.* This perceived drawback is not valid - if anything, RIP's approach will require the least number of simulations. In any stochastic analysis based on sampling, it is necessary to analyze a large number of samples if the 'tails' of the system probability distribution are to be evaluated. However, the number of samples required is essentially independent of the degree of complexity of the system, and depends only on how precise the probability distribution needs to be. Approaches based on separate stochastic analyses of a number of scenarios will require each scenario to be sampled repeatedly, and the results aggregated, so the overall number of simulations will be higher than with RIP's approach. Approaches based on deterministic analysis of a number of scenarios could not produce defensible probability distributions unless the number of scenarios is very large. Approaches based on deterministic, worst-case scenarios may be overly conservative, in which case a good repository would be discarded, or may founder in debate over whether they are truly a worst case.

It is important to note that a repository system does not have a finite number of discrete states: it entails a large number of continuously-varying stochastic parameters. Approaches based on 'tree'-type logic diagrams are very useful in developing an understanding of the kinds of processes that may occur, but unfortunately will not lead directly to a valid probability-tree approach to scenarios.

RIP minimizes the number of simulations required by using two separate 'importance sampling' techniques, as discussed in Appendix C. RIP does not sample all possible systems equally: it can sample certain realizations more frequently than others. The resulting probability distributions of performance are corrected to compensate for the bias in sampling. The result is that higher accuracy in the system probabilities is achieved with fewer simulations. RIP's two importance-sampling techniques are 1) selectively enhanced sampling of system histories where disruptive events occur; and 2) selectively enhanced sampling nearer to the extremes (tails) of parameter distributions. RIP also incorporates a stratified (Latin-Hypercube) sampling scheme to further enhance the sampling efficiency.

- *The model will become impossibly complex.* There is a trade-off here: because RIP attempts to simulate all possible system behaviors, it is a sort of 'jack of all trades

and master of none'. RIP has to use simplified sub-models, and the price is in an increased level of model error. In principle, the data input to RIP will be based on 'detailed' external models of components of the system, but within RIP these models may be represented by interpolation tables or curve-fits to response surfaces. It is conceivable that the performance assessment model eventually required for a license application will be more like an orchestra leader, where a driving program will invoke one or more of a suite of specialized simulators as required by the specific realization.

RIP's rather direct approach has the benefit of avoiding the problems associated with defining 'mutually exclusive' scenarios. Since RIP encompasses all futures within what is essentially a single scenario, the issue does not arise. Also, RIP avoids the issue of aggregating a set of scenarios (a 'scenario group') into an archetypical scenario. Any set of archetypical scenarios may be criticized as not being adequately refined: perhaps a slightly different combination of timing or magnitudes would produce different results. With RIP, refinement (discretization) is an automatic process, and is based only on computing an adequate number of simulations. Finally, RIP will automatically create 'combined' events or scenarios if they are credible, simply by its random sampling logic, avoiding another difficulty with scenario-driven methods.

References

DOE 1988, Site Characterization Plan, Section 8.3.5.13, U.S. Department of Energy, Office of Civilian Radioactive Waste Management, December, 1988

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APPENDIX C

ENHANCED SAMPLING TECHNIQUES AND COMPUTATION OF CONFIDENCE BOUNDS

The RIP program has the ability to display the results of a Monte Carlo simulation as a cumulative distribution function (CDF), a complimentary cumulative distribution function (CCDF), or a probability distribution function (PDF). For computational simplicity RIP may not store all the results generated, and the first part of this section explains how the results of a Monte Carlo simulation are stored and displayed within RIP.

The EPA's 40CFR191 regulation stipulates that a high-level nuclear waste repository must be demonstrated to "Have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1". For a Monte Carlo-based performance-assessment model such as RIP, this implies that runs involving 10,000 or more realizations would be required. In order to get a reasonably accurate estimate of the 0.999 quantile of a result, as required by 40CFR191, as many as 100,000 realizations may be required. Even with a very fast, simple model which took just one second to evaluate a realization, 100,000 realizations would take over a day to perform. Thus, it is important to seek ways to decrease the number of realizations required to reach a certain desired accuracy.

RIP can minimize the number of Monte Carlo simulations required to construct a CCDF by using two separate 'importance sampling' techniques. These techniques work so that RIP does not sample all possible systems equally: it samples certain realizations more frequently than others. The resulting probability distributions of performance are corrected to compensate for the bias in sampling. The result is that higher accuracy in the system probabilities is achieved with fewer simulations. RIP's two importance-sampling techniques are 1) selectively enhanced sampling of system histories where disruptive events occur, and 2) selectively enhanced sampling nearer to the extremes (tails) of parameter distributions.

After explaining how results are stored and displayed within RIP, this appendix discusses the mathematical basis of each of the two importance-sampling methods, and presents numerical results demonstrating their effectiveness.

In addition to importance sampling, RIP offers the user an option of conventional or Latin-Hypercube sampling of stochastic parameters. The Latin-Hypercube option, described in Section C.3, offers some additional advantages over conventional Monte Carlo sampling.

Section C.4 discusses how confidence bounds on the resulting PDFs, CDFs, and CCDFs are computed, based on the number of realizations carried out, and the nature of the sampling technique.

C.1 Creation of a CDF

The RIP program generates Monte Carlo realizations, both for individual stochastic parameters and for full probabilistic assessments. The results of these Monte Carlo realizations may be viewed in the form of a CDF (or a CCDF). This section describes how the values realized during the simulations are used to generate the CDF (or CCDF) seen by the user.

C.1.1 Creating the Results Array

Within RIP Monte Carlo results are stored in a particular data structure, referred to here as the "results array". As the simulation progresses, each specific Monte Carlo realization result is added to the results array as a pair of values; the value realized and the weight given by RIP to the value. The array is filled "on the fly", as each new realization is generated. Theoretically, each separate realization would represent a separate entry in the results array (consisting of a value and a weight). If unbiased sampling were carried out each separate entry would have equal weight.

As implemented in RIP, however, the number of data pairs in the results array may be less than the number of realizations: There are two reasons why this may be the case:

- If multiple results have identical values, there is no need to have identical data pairs in the results array: the weight associated with the particular value is simply adjusted (e.g., if the value occurred twice, its weight would be doubled).
- For computational reasons, the results array has a maximum number of unique results which it can store. The maximum number for post-processing RIP simulation results is 5000; the maximum number for viewing stochastic parameters (using the F7 key in the parameters module) is 1000. If the number of realizations exceeds these limits, results are "merged" in a self-consistent manner. The process of merging results when the number of realizations exceeds 5000 (or 1000) is discussed below.

To merge a new result with the existing results (in cases where the number of realizations exceeds one of the maxima specified above), RIP carries out the following operations:

- 1) RIP finds the surrounding pair of existing results, and selects one of them to merge with. RIP selects this result based on the ratio of the distance to the result to the weight of the result (i.e., the program preferentially merges with closer, lower weight results).
- 2) After selecting the result to merge with, RIP replaces its value with the weighted average of its existing value and the new value; it then replaces its weight with the sum of the existing and new weights.

There is one important exception to the merging algorithm discussed above: If the new result will be an extremum (i.e., a highest or a lowest), RIP replaces the existing extremum with the new one, and then merges the existing result instead. This means that RIP never merges data with an extremum.

C.1.2 Plotting the CDF

Plotting the CDF from the results array is straightforward. The basic algorithm assumes that the probability distribution between each adjacent pair of result values is uniform, with a total

probability equal to half the sum of the weights of the values. One implication of this assumption is that for a continuous distribution the probability of being less than the smallest value is simply equal to half the weight of the lowest value and the probability of being greater than the highest value is half the weight of the highest value.

For example, if we have ten equally weighted results in a continuous distribution, there is a uniform probability, equal to 0.1, of being between any two values. The probability of being below the lowest value or above the highest value would be 0.05. For this example, RIP would only plot the CDF (or CCDF) between the ranges of 0.05 and 0.95. RIP does not attempt to extrapolate beyond the lowest and highest actual results, and truncates the CDF (or CCDF) vertically at these points.

In certain circumstances there are several minor variations to the basic algorithm discussed above:

- 1) If the number of distinct results is much smaller than the number of realizations, RIP assumes the distribution is discrete (rather than continuous), and lumps the probabilities at the actual values sampled. In particular, if the total number of unique results is ≤ 20 , and more than 50% of the realization results were identical to an existing result, RIP presumes the distribution is discrete and plots it accordingly. The user can observe this by sampling from a binomial distribution.
- 2) RIP uses a heuristic algorithm to decide if each specific result represents a discrete value: if the number of exact repetitions of a particular result exceeds $2(1 + \text{average number of repetitions})$, RIP treats the result as a discrete value and does not 'smear' it. For example, suppose the result is 0.0 50% of the time, and normal (mean=10, s.d.=2) the rest of the time. The first result value would be 0.0, with a weight of about 0.5. The second value would be close to 8, with a weight of $1/\#$ realizations. We would not want to smear half of the 0 result over the range from 0 to 8!

Note that the main parameter display window only shows 11 (value, cumulative probability) pairs. A larger number of pairs can be written the screen (or a data file) using the F5 key, such that the distributions can be manipulated and plotted outside of RIP.

C.1.3 Viewing the Raw Data

The results array and the computed cumulative probability levels can be viewed by hitting F3 and then ENTER from the parameter display window (hitting ENTER rather than a filename sends the data directly to the screen).

C.2 Importance-Sampling of Events

Because RIP represents disruptive events as Poisson processes, it is not appropriate to do performance-sampling of events by simply increasing the rate of occurrence of the events. For example, having volcanoes erupt every year, but with a low 'weight', is physically unreasonable.

Instead, RIP uses a 'pruning' process to selectively discard a fraction of the less-important realizations. As a simple example, the user could choose to model every realization which involved a volcanic event, but to discard nine out of ten non-volcano realizations. RIP automatically carries out this pruning, and corrects the resulting CCDFs by weighting the resulting realizations inversely by their pruning factor. That is to say, if a particular event-class was pruned nine times out of ten, then for each realization that was retained the result would be processed as if it had occurred ten times.

The following table shows an example of this approach.

Sampling Class	Fraction Kept (un-pruned)	Class Criteria	Weight Applied (Pruning Factor)
I	1	Volcano or Earthquake	1
II	0.4	Human Intrusion Events	2.5
III	0.1	All others	10

Table C.1 Example Event-Pruning Table

The benefit of this approach is that unusual events will be sampled much more frequently than under the normal Monte Carlo approach, and so their likelihood and consequences will be represented much more precisely in the resulting CCDFs.

For example, suppose that volcanic events normally occur at a rate of one every 10,000,000 years. For 10,000-year simulations, a volcanic event would normally occur only once every 1,000 realizations. A Monte Carlo simulation using 1,000 realizations would have only a 0.63 likelihood of realizing one or more volcanic events, and therefore would have an extremely poor representation of volcanic events in its CCDF. Importance sampling where volcanic events were selected ten times more frequently than other cases would on average result in ten volcanic events over a thousand realizations: enough for a rough approximation of their effects. More realizations, or a higher selectivity of volcanic events, would produce an even better result.

It should be noted that there can be too much of a good thing, and excessive pruning of the base case would result in degradation of the base-case portion of the CCDF, so that the computed expected value or first moment of the distribution would be poor. For example, a pruning-factor of 1000 in the above example for "all others" would have resulted in only one in a thousand realizations of the base case being retained. This clearly would be too few.

The RIP user defines event importance-sampling in a simple manner. Similarly to the preceding table, the user creates event-classes, which jointly span all possible histories. Each event class is given a pruning factor, and a list of which events define each class. The pruning and weighing operations are performed automatically by RIP.

As a simple demonstration of event importance-sampling, a system was defined whose 'base-case' performance was represented by a normal distribution with mean 0 and standard deviation 1. Two events were defined, as follows:

- Event 1 had an expected number of occurrences equal to 0.01, with the consequence having a normal distribution with a mean of 4 and a standard deviation of 0.4,
- Event 2 had an expected number of occurrences of 0.001, with the event consequence having a mean of 10 and a standard deviation of 1.

In each case, if the event occurred then the event consequence was added to the base-case consequence. This system was sampled 1,000 times using pruning-factors of 1, 10, and 100 for the base case, with the resulting density functions shown in Figure C-1. For comparison, the result of a conventional Monte Carlo analysis using 10,000 realizations is shown. Note the low probability occurrences of multiple events apparent in the figure. As can be seen, the importance-sampling approach radically improved the ability of the Monte Carlo method to represent the consequences of low-likelihood events.

C.3 Importance-Sampling of Tails of Distributions

C.3.1 Theory

In the Monte Carlo simulation process, each random variable is normally sampled purely randomly or by Latin-hypercube sampling. However, in performance assessment the area of interest is usually the extreme tail of the results distribution. In order to increase the resolution of the tails for a given number of system realizations, RIP uses an importance-sampling technique which can sample the extremes of the random variables at an enhanced rate. To counteract the increased sampling rate, a sampling weight is calculated for each variable, where the weight is inversely proportional to the degree of sampling enhancement. Each realization of the entire system has a weight equal to the product of the weights of the individual, independent stochastic parameters.

For a random variable x with probability density $f(x)$, normal Monte Carlo sampling will yield a sample within the range $(x, x+dx)$ about $f(x)dx$ fraction of the time, for a large number of samples and a small dx . In the importance sampling scheme, a sample in the range $(x, x+dx)$ is generated $b(x)f(x)dx$ fraction of the time, with an associated weight of $1/b(x)$. $b(x)$ is termed the 'bias function' in RIP.

In the conventional Monte Carlo process, a random number ' r ' is selected from the uniform distribution $(0,1)$, and is used as the probability level in the cumulative distribution function $F(x)$. Thus, the normal Monte-Carlo selection is $x = F^{-1}(r)$.

RIP transforms r to ' u ', the 'used' random number, as follows:

$$u = 0.5 (2r)^n$$

where n (n greater than or equal to 1) is a factor that controls the extent of the biasing towards the tails. The weight associated with $F^{-1}(u)$ is simply du/dr :

$$w = du/dr = n(2r)^{n-1}$$

Note that this approach amplifies both tails of the probability distribution equally. This is because we do not know ad hoc which tail is of the most interest. The form selected for u is not very strong, and there may be cases where a transformation which is stronger, or which amplifies just the upper (or lower) end of the distribution would be preferred.

Graphically, we are simply transforming r into u , as shown in Figure C-2.

The following table of u and w shows how the amount of biasing changes with different values of n :

	r=0.01		r=0.1		r=0.5	
n	u	w	u	w	u	w
1	0.01	1	0.1	1	0.5	1
1.33	0.0028	0.3658	0.0588	0.7820	0.5	1.33
1.67	0.0007	0.1215	0.0340	0.5681	0.5	1.67
2.0	0.0002	0.0400	0.0200	0.4000	0.5	2.0

Table C.2 Values of the 'used' random number u and its weight w .

where:

- n = the bias exponent
- r = the original random number which was selected
- u = the 'used' random number
- w = the weight

Note: the table does not show values of $r > 0.5$, as the weighing is symmetrical about $r = 0.5$.

The net effect of the importance-sampling technique is to develop relatively more realizations at the ends of the probability distributions. Where the goal is to develop an accurate measure of the cumulative probability at a very high consequence level, this technique should reduce the number of realizations required.

In RIP, any stochastic variable can be assigned an importance-sampling bias factor, using the terminology 'low bias' for $n = 1.33$, 'medium bias' for $n = 1.67$, and 'high bias' for $n = 2$.

C.3.2 Test Problem

A test was carried out involving realizing the function $y = x_1 + x_2 e^{x_3}$ a thousand times. The input parameters were defined as follows: x_1 had a normal distribution with mean 5 and standard deviation 2, x_2 had a normal distribution with mean 1 and standard deviation 0.5, and x_3 had a triangular distribution with lower bound 0, upper bound 3, and most likely value 1.

The resulting distribution of y was sampled at a number of probability levels. The entire process was repeated twenty times, and the statistics of the resulting distributions of the sampled quantiles were calculated. This was done for two different values of the biasing parameter, n : $n = 1$ (no biasing), and $n = 2$ (high biasing). The results, as shown in Figure C-3, demonstrate a dramatic improvement in the tails at the higher value of n . For comparison, the result using Latin-Hypercube sampling (without any importance sampling) are also shown.

C.4 Latin-Hypercube Sampling (LHS)

RIP also presents an option to implement a Latin-Hypercube sampling (LHS) scheme. The LHS option results in forced sampling from each "stratum" of a parameter. The parameter's distribution is divided into up to 250 equally likely strata or slices. The strata are then "shuffled" into a random sequence, and a random value is then picked from each stratum in turn. This approach ensures that a uniform spanning sampling is achieved.

The number of strata used is the largest whole number, less than 251, that will equally divide into the number of realizations. Where more than 250 realizations are specified, sets of strata are defined as shown in examples in the following table:

Number of LHS Strata		
# of realizations	# of sets	# of strata per set
100	1	100
200	1	200
250	1	250
251	2	126
1000	4	250
3333	14	239

Table C.3 Latin-Hypercube Strata

When more than one set of strata are used, each parameter is randomly re-positioned in its sampling sequence after each set is completed.

LHS appears to have a significant benefit for problems involving only a few independent stochastic parameters, and with moderate numbers of realizations. In no case does it perform worse than true random sampling, and accordingly LHS sampling is the default for RIP.

Note that Latin-Hypercube sampling is not meant to be an alternative to importance sampling. Rather, importance sampling can be implemented simultaneously with Latin-Hypercube sampling to further augment the sampling scheme. In general, Latin-Hypercube sampling is effective at delineating the base-case portion of a stochastic result (i.e., the expected value or first moment). It is not efficient at sampling the tails of distribution. Importance sampling, however, is designed to effectively sample the low probability tails. Hence, a combined Latin-Hypercube/importance sampling scheme is likely to be the most efficient sampling approach. Sampling schemes are discussed in more detail in the RIP User's Guide.

C.5 Confidence Bounds on Monte Carlo Results

RIP is able to perform a statistical analysis of Monte Carlo results to produce confidence bounds on the resulting probability distribution curves. These bounds reflect uncertainty in the probability distribution due to the finite number of Monte Carlo realizations - as the number of realizations is increased, the limits become narrower.

The confidence bounds (which may take a second or so to calculate) appear as different-colored curves on the probability plots produced by the RIP user interface. For CDFs (Cumulative Distribution Functions) and CCDFs (Complementary Cumulative Distribution Functions), the bounds represent 5% and 95% confidence limits on the distribution value at each probability level. For probability density plots, the bounds represent 5% and 95% confidence bounds for the average probability density over each plotted "bin". Figures C-4 and C-5 illustrate the bounds calculated for a triangular probability distribution which was sampled 200 times.

The theory used to produce the confidence bounds has several limitations:

- The bounds on CDF and CCDF distributions can only be calculated for cases where all realizations have equal weights. If importance sampling is used for any parameter, or if event-pruning is used, RIP will not display confidence bounds on CDF and CCDF plots.
- The CDF and CCDF confidence bounds cannot be calculated for values less than the smallest result, or greater than the largest result. As a result of this, the confidence-bound curves do not generally reach all of the way to the tails of the result plots.
- In cases with relatively few stochastic parameters, Latin Hypercube sampling can increase the accuracy of the probability distributions. The confidence bounds are not able to reflect this improvement, and as a result will be conservatively wide in such cases.

C.5.1 Theory: Bounds on Cumulative Probability

Suppose we have calculated and sorted in ascending order n random results r_i from a distribution. What can we say about the q^{th} quantile x_q (e.g., $q=0.9$) of the underlying distribution?

Each random result had a probability of q that its value would be less than or equal to the actual q^{th} quantile x_q . The total number of results less than x_q was therefore random and binomially distributed, with the likelihood of exactly i results $\leq x_q$ being:

$$P(i) = P(r_i \leq x_q \leq r_{i+1}) = \binom{n}{i} q^i (1-q)^{n-i} = \frac{n!}{i!(n-i)!} q^i (1-q)^{n-i} \quad (\text{C-1})$$

Note that there may be a finite probability that the value of x_q is less than the first or greater than the largest result: for example, if 100 realizations r_i were sampled, there would be a probability of 0.366 that the 0.99 quantile exceeded the largest result. The 100 realization probability distribution for $x_{0.99}$ is as follows:

Between Results	Probability	Cumulative Probability
<94	0.0000	0.0000
94 and 95	0.0005	0.0005
95 and 96	0.003	0.0035
96 and 97	0.015	0.0185
97 and 98	0.061	0.0795
98 and 99	0.1849	0.2644
99 and 100	0.370	0.6344
>100	0.366	1.

Table C.4 Probability Distribution for Location of actual 0.99 Quantile within a set of 100 Realized Results

RIP assumes that the probability defined by Equation C-1 is uniformly distributed over the range from r_i to r_{i+1} , and interpolates into the Monte Carlo results-list to find the 5% and 95% cumulative probability levels for x_q . For example, for 100 realizations, the 5% confidence bound on the 0.9 quantile is 0.31 of the distance from result 85 to result 86, and the 95% confidence bound is 0.22 of the distance from result 95 to result 96.

Between Results	Probability	Cumulative Probability
<85	-	0.040
85 and 86	.033	0.073
86 and 87	0.051	0.124
87 and 88	0.074	0.198
88 and 89	0.099	0.297
89 and 90	0.120	0.417
90 and 91	0.132	0.549
91 and 92	0.130	0.679
92 and 93	0.115	0.794
93 and 94	0.089	0.883
94 and 95	0.060	0.942
95 and 96	0.034	0.976
96 and 97	0.016	0.992
97 and 98	0.006	0.998
98 and 99	0.0016	1.000
99 and 100	0.000	1.000
>100	0.000	1.000

Table C.5 Probability Distribution for Location of actual 0.9 Quantile within a set of 100 Realized Results

Using the above probability distribution, it is also possible to calculate the expected value of x_q . This approach appears (by experimentation) to provide a slightly more reliable estimate of x_q than the conventional Monte Carlo approach of directly interpolating into the results-list. The expected value of x_q is calculated by summing the product of the probability of x_q lying between each pair of results and the average of the corresponding pair of result-values, i.e.,

$$\bar{x}_q = \sum_{i=1}^n P(i) \frac{[r_{i+1} + r_i]}{2} \quad (C-2)$$

When using Equation C-2 to estimate a very high or low quantile, a problem arises when the probability level, q , is near to 0 or 1, as there can be a significant probability that x_q lies outside the range of results. In Table C-1, for example, there is a 0.366 chance of $q_{0.99}$ exceeding the largest result. In such cases, an estimate of the expected value of x_q can be found by

extrapolating from the probabilities within the range of the results. Obviously, however there are limits to extrapolation and without knowledge of the actual distributional form no extrapolation would produce a reliable estimate of (say) the 0.9999 quantile if only 100 realizations had been performed.

In evaluating the binomial distribution for large values of n , large numbers can be generated which can cause numerical difficulties. To avoid these difficulties, when the number of realizations (n) is greater than 100, RIP uses either the normal or Poisson approximations to the binomial distribution. The Poisson approximation is used when i or $(n-i)$ is less than 20 and the normal distribution is used otherwise. These approximations are described in any introductory statistics text

C.5.2 Theory: Bounds on Probability Density

For calculating bounds on the probability density, RIP evaluates the statistics of the number of results falling into specific "bins". The range of results from r_1 to r_n is divided into a user-definable number of equal-width bins (RIP assigns a default number of bins, based on the number of realizations). The probability-density computed for each bin is calculated as the estimated fraction of all results which fall in the bin divided by the bin-width.

If, in a Monte Carlo simulation, i out of n realizations fell into bin j , what is the probability distribution for the actual fraction F_j of the underlying distribution that falls in the j^{th} bin? The number of realizations in the j^{th} bin is binomially distributed:

$$P(i \text{ results in bin } j) = \binom{n}{i} F_j^i (1 - F_j)^{n-i} = \frac{n!}{i!(n-i)!} F_j^i (1 - F_j)^{n-i} \quad (\text{C-3})$$

Not knowing F_j in advance, and observing that i out of n realizations fell in bin j , the probability density for F_j is proportional to the relative likelihood of observing i out of the n realizations, as shown in Equation C-3, as a function of F_j . This is simply the beta distribution, $\beta(i-1, n-i-1)$, whose cumulant is the incomplete beta function. For example, if 10 out of 100 realizations fell into a particular bin, the distribution of F_j would be as shown in Figure C-6.

The accuracy of the estimated probability density decreases as the bins are made smaller, because there are fewer results in any particular bin. Thus, the RIP user has to choose between large bins which will give a more precise estimate of their average probability density, but which may obscure details of the distribution form, and small bins which will have a larger amount of random error. The user can experiment with this effect by altering the desired number of bins prior to plotting.

RIP can calculate confidence bounds for PDFs even when using importance sampling or pruning. A heuristic approach is taken, whereby an 'effective' total number of realizations n_e is used rather than the actual number n . The 'effective' number is calculated by scaling the actual number of realizations so that the average realization weight is the same for the overall set of results as for the bin being evaluated, i.e. $n_e = (n_{\text{bin}})(w_{\text{total}})/w_{\text{bin}}$. Thus, if the bin had a high

proportion of low-weight results, n would be increased as if the sampling had been from a population with a similarly high proportion of low-weight results.

For discrete-valued distributions that same approach applies, and Equation C-3 can be directly applied to find confidence bounds on the fraction of the population having a particular value.

C.5.3 Limits Due to RIP's Method of Saving Monte Carlo Results

When carrying out a RIP simulation involving large numbers of realizations, the amount of computer-memory allocated to saving the Monte Carlo results can become excessive. Accordingly, RIP limits the amount of memory allocated to storing results (based on the amount of memory available), and in any event never stores more than 5,000 different results per parameter. For larger numbers of realizations, RIP will automatically 'blend' neighboring results, keeping track of the combined count and 'weight' of each result. The lowest and highest results are never blended. The resulting set of blended results is an approximation of the actual results. By and large, this process is invisible to the user and has no deleterious effects on the accuracy.

FIGURE **C-1**
EVENT IMPORTANCE
SAMPLING - RESULTS
 ARGONNE/MODEL DEVELOPMENT/WA

FIGURE **C-2**
PARAMETER IMPORTANCE - SAMPLING ALGORITHM
 ARGONNE/MODEL DEVELOPMENT/WA

FIGURE **C-3**
PARAMETER IMPORTANCE
SAMPLING - RESULTS
 ARGONNE/MODEL DEVELOPMENT/WA

Results for parameter TR012, 200 realizations

FIGURE **C-4**
 MONTE CARLO RESULT DISTRIBUTION
 SHOWING CONFIDENCE BOUNDS

Results for parameter TR012,

200 realizations

— Mean — 0.05, 0.95 confidence limits

Results of 200 Monte Carlo realizations.

Mean= 0.9878

S.D.= 0.4126

FIGURE **C-5**
MONTE CARLO RESULT DENSITY
SHOWING CONFIDENCE BOUNDS

Result for stochastic parameter ABETA

Beta Distribution

Mean= 1.000E-01

S.D.= 2.985E-02

FIGURE **C-6**
BETA DISTRIBUTION OF F_j ,
THE ACTUAL FRACTION IN BIN $_j$

APPENDIX D

RADIOACTIVE DECAY ALGORITHM

This appendix explains the general algorithm for radioactive decay used in the RIP model. We begin by considering the mass balance for a single radionuclide in a closed system. This equation is given by:

$$\frac{dM_i}{dt} = -\lambda_i M_i + \sum_j^k \lambda_j M_j \quad (D-1)$$

where

M_i is the mass of the i th radionuclide,
 M_j is the mass of the j th parent to radionuclide i ,
 $\lambda_{[i,j]}$ is the radioactive decay constant for the i th or j th radionuclide, and
 t is time

In the RIP model, we solve Equation D-1 for M_i at time t using a backward difference approximation for the derivative. Replacing dt with Δt , equation D-1 is solved for $M_i(t)$ as follows:

$$M_i(t) \approx (1 - \lambda_i \Delta t) M_i(t - \Delta t) + \Delta t \sum_j^k \lambda_j M_j(t - \Delta t) \quad (D-2)$$

where

$M_i(t)$ is the mass of the i th radionuclide at time t , and
 $M_i(t - \Delta t)$ is the mass of the i th radionuclide at time $t - \Delta t$.

The approximate solution for $M_i(t)$ given by equation D-2 has error of order Δt . The actual error is also influenced by the radioactive decay constant. For small decay constants (long half-lives), a larger value of Δt may be used than for more rapidly decaying radionuclides. RIP applies Equation D-2 using a sub-time step Δt equal to 1/1024 of the RIP time step.

For a large inventory of radionuclides, including decay chains of several members in length, it is convenient to write the individual equations D-2 as a linear system. The linear system used to compute $M(t)$ is given by the following:

$$M(t) \approx [D] M(t - \Delta t) \quad (D-3)$$

where

$[D]$ is a coefficient matrix,
 $M(t - \Delta t)$ is the radionuclide mass vector at time $t - \Delta t$, and
 $M(t)$ is the radionuclide mass vector at time t .

The matrix elements of $[D]$ are given by:

$d_{ij} = 1 - \lambda_i \Delta t$, if $i = j$
 $d_{ij} = \lambda_j \Delta t$, if $i < > j$ and j is a parent of i , and
 $d_{ij} = 0$, if $i < > j$ and j is not a parent of i .

In executing the RIP model, radionuclide decay calculations are made at every time step. The time step size is likely to be 100 years or larger for most long-term simulations.

A preprocessing step in the RIP algorithm computes the matrix $[D]$. Decay is then computed at each later time step by carrying out the matrix multiplication $[D] M(t-\Delta t)$ to obtain $M(t)$.

RIP calculates a decay-matrix $[D]$ for an entire RIP time step by successively squaring the decay matrix for the sub-time step. The initial decay matrix $[D]_{1024}$ is calculated for a time step equal to $1/1024$ of the RIP time step. This matrix is then squared ten times:

$[D]_{1024}^2 = [D]_{512}$, the decay matrix for $1/512$ of the RIP time step. $[D]_{512}^2 = [D]_{256}$, the decay matrix for $1/256$ of the RIP time step, $[D]_{256}^2 = [D]_{128}$, $[D]_{128}^2 = [D]_{64}$, and so on. The resulting $[D]$ matrix provides an extremely accurate estimate of the decay, even for very short-lived isotopes.

Note that the current algorithm does not allow a parent to split more than one daughter. That is, a daughter can have more than one parent, but a parent can have no more than one daughter.

APPENDIX E

COMBINING WASTE PACKAGE FAILURE MODE DISTRIBUTIONS

In Chapter 3, waste package failure models of the RIP model are discussed in detail. Generally, the failure models for either primary or secondary containers include more than one failure mechanism, or mode. This appendix presents the derivation of the failure model used in RIP, which consists of a combination of one or more modes.

Let

- N = number of failure model;
- $f_i(t)$ = frequency of failure by mode i at time t ;
- $F_i(t)$ = probability of failure by mode i by time t ;
- p_i = fraction of waste packages which can fail by mode i ;
- $f(t)$ = frequency of failure by all modes combined at time t ; and
- $F(t)$ = probability of failure by all modes combined by time t .

By definition,

$$F_i(t) = \int_0^t f_i(\theta) d\theta \quad (E-1)$$

and

$$F(t) = \int_0^t f(\theta) d\theta \quad (E-2)$$

We would like to develop an expression such that the combined distributions $f(t)$ and $F(t)$ can be expressed in terms of the distributions for the modes, $f_i(t)$ and $F_i(t)$. The derivation is straightforward.

$$1 - p_i F_i(t) = \text{probability of surviving mode } i \text{ by time } t \quad (E-3)$$

Assuming that the failure modes are uncorrelated, it follows that

$$\prod_{i=1}^n [1 - p_i F_i(t)] = \text{probability of surviving all modes by time } t \quad (\text{E-4})$$

and

$$F(t) = 1 - \prod_{i=1}^n [1 - p_i F_i(t)] = \text{probability of not surviving all modes by time } t \quad (\text{E-5})$$

In the RIP model, only $F(t)$ is used in the calculations. Where needed, $f(t)$ is approximated by $[F(t) - F(t-\Delta t)]/\Delta t$. This approximation ensures the pdf integrates to 1, as required. This approximation eliminates balancing errors which may occur due to a poor approximation of $f(t)$ over the interval $(t, t + \Delta t)$.

APPENDIX F

USING THE EXPONENTIAL, WEIBULL, AND OTHER DISTRIBUTIONS

TO REPRESENT WASTE PACKAGE FAILURE

Primary and secondary container failure rates will be obtained from probability density functions. The failure rates of either containers or cladding will be based on estimated probability density functions for the lifetime of containers and the lifetime of cladding. The failure rates at any time during a simulation are equal to the lifetime probability density function value at that time.

The use of the five available distribution types for describing container failure (exponential, weibull, uniform, degenerate, and log-uniform) is discussed below.

Exponential Distribution

The exponential distribution is fully described by a single parameter. This parameter, λ , is the inverse of the expected lifetime and appears in the exponential probability density function (pdf) as follows:

$$f(t) = \lambda e^{-\lambda t} \quad t \geq 0, \lambda > 0 \quad (F-1)$$

Where the random variable t is the lifetime (Hogg and Craig, 1978). The mode of the exponential distribution always occurs at $x = 0$, and the variance is equal to the square of the expected value. Hence, the expected value and standard deviation are also equal.

The value of $f(t)$ is the frequency of lifetimes equal to t . Thus, in a population of canisters of size N , we expect $Nf(t)dt$ of the containers to be breached in a time interval from t to $t+dt$. Hence, $f(t)$ is a failure rate for time interval dt . Likewise, for a container containing N_r spent fuel rods we expect $N_r \times f(t)dt$ of the rods to be breached (i.e., undergo cladding failure) in the time interval from t to $t+dt$. Figure F-1 shows Equation F-1 for various values of λ .

The determination of λ may be simplified by considering the cumulative probability density function (cdf), which is given as follows:

$$F(t) = 1 - e^{-\lambda t} \quad t \geq 0, \lambda > 0 \quad (F-2)$$

The cdf relates a total fraction to a time given a value of λ . For example, if a project scientist can estimate that 50% of the containers will be breached in 1,000 years due to engineered and/or handling related defects, λ can be solved for directly from Equation F-2. For this example,

$$1 = \frac{-\ln(0.5)}{1000} = 0.000693 \text{ yr}^{-1} \quad (F-3)$$

To aid this elicitation procedure, it is also worth noting that 63% of the canisters will be breached at the expected lifetime, 86% at a time equal to twice the expected lifetime, and 95% at a time equal to three times the expected lifetime. This procedure may be used to obtain bounds on the range of λ .

Weibull Distribution

The Weibull distribution is more complex than the exponential distribution, requiring the input of three parameters rather than one. The pdf for the Weibull distribution is given as follows:

$$f(t) = \frac{\alpha}{\beta - \varepsilon} \left(\frac{t - \varepsilon}{\beta - \varepsilon} \right)^{\alpha-1} e^{-\left(\frac{t - \varepsilon}{\beta - \varepsilon} \right)^\alpha} \quad (F-4)$$

$$t \geq \varepsilon, \beta > \varepsilon, \alpha > 0$$

where the random variable t is the lifetime (Benjamin and Cornell, 1970). The parameter ε is a minimum lifetime value at which $f(t) = 0$. The expected and model value of t are proportional to β , while the variance of t is proportional to β^2 . The parameter α relates to the shape of $f(t)$ and influences the expected value, variance and mode.

The expected value and variance of t in the Weibull distribution are given as follows:

$$E(t) = \varepsilon + (\beta - \varepsilon) \Gamma\left(1 + \frac{1}{\alpha}\right) \quad (F-5)$$

$$\text{Var}(t) = (\beta - \varepsilon)^2 \left[\Gamma^2\left(1 + \frac{2}{\alpha}\right) - \Gamma^2\left(1 + \frac{1}{\alpha}\right) \right]$$

The most probable value of t , or distribution mode, is give by:

$$\text{MODE}(t) = \varepsilon + (\beta - \varepsilon) \left(\frac{\alpha - 1}{\alpha} \right)^{\frac{1}{\alpha}} \quad \alpha > 1 \quad (F-6)$$

$$\text{MODE}(t) = 0 \quad \alpha \leq 1 \quad (F-7)$$

(Benjamin and Cornell, 1970).

Figure F-2 shows Equation F-4, for various values of α , when $\beta = 5,000$ years and $\varepsilon 1,000$ years. As α increases from 0.5 to 7 the distribution form shifts from that similar to the exponential function to a more bell-shaped curve. In fact, for $\alpha = 1$, the Weibull pdf reduces to the exponential pdf discussed above with $\lambda = 1/(\beta - \varepsilon)$. As alpha continues to increase to $+\infty$, $f(t)$ becomes a spike centered very close to β . For large values of α , the variance of t asymptotically approaches 0, causing the distribution to become essentially degenerate.

Figure F-3 shows the behavior of the mean (expected value), variance, and mode of lifetimes following the Weibull distribution, as functions of the parameter α . The ordinate axis, labeled parameter weightings, provides the values of the right-hand sides of Equations F-5 and F-6 when they are arranged to contain only the parameter α .

It is important to note from these curves, that the mode and mean are equal only when $\alpha = 3.345$. When $\alpha = 3.345$ the mean value is equal to $\varepsilon + (\beta - \varepsilon)0.898$. To the left of $\alpha = 3.345$, the mode occurs to the left of the mean, whereas to the right of $\alpha = 3.345$, the mode occurs to the right to the mean. For values of $\alpha > 1$, the lifetime variance rapidly approaches 0.

The elicitation of the Weibull distribution parameters may likely be pursued in many ways. One method for their elicitation is the following:

- 1) Determine ε independently from α and β . ε represents the first possible time of failure due to conditions in the repository. Consequently, it can be interpreted as independent of α and β .
- 2) Determine the distribution of α with the aid of Figure F-3. Based on the desired population of distribution shapes, a distribution for α may be estimated.
- 3) Evaluate the distribution of mean lifetime assuming $\varepsilon = 0$. A mean lifetime distribution for $\varepsilon > 0$ may be obtained by adding ε to the mean when $\varepsilon = 0$. The difference, $\beta - \varepsilon$, which fully determines the Weibull distribution, is obtained from the mean lifetime using Equation F-8 below.

$$\beta - \varepsilon = \frac{E(t, \varepsilon = 0)}{\Gamma(1 + \frac{1}{\alpha})} \quad (F-8)$$

Uniform Distribution

The uniform distribution is usually described by two parameters, a and b , which define the interval of the random variable over which the distribution has a density greater than 0. The probability density for any value of the random variable within the closed interval $[a, b]$ is equal to $1/(b-a)$, as shown on Figure F-4. Although the uniform distribution is conventionally not described in terms of its mean and variance, these statistics are equal to $(b+a)/2$ and $(b-a)^2/12$, respectively.

With respect to container, we have chosen to define the uniform distribution in a slightly different but equivalent manner. Rather than specifying the interval endpoints, we specify the first possible lifetime, equivalent to the parameter a , and then the duration of positive probability density. This duration is equivalent to the difference $b-a$. These two parameters fully define the uniform distribution.

Log-Uniform Distribution

The log-uniform distribution is used when the logarithm of the random variable (in this case the failure time) is described by a uniform distribution. The distribution requires a start time and a duration. Note that the start time must be greater than 0 (since the log of 0 is undefined). The pdf of a log-uniform distribution is given as follows:

$$f(x) = \frac{1}{x \left[\ln \left(\frac{b}{a} \right) \right]} \text{ for } a \leq x \leq b \quad (\text{F-9})$$

where a is the start time and $b = \text{start time} + \text{duration}$.

Degenerate Distribution

The degenerate distribution has all its probability density concentrated at a single value of the random variable, i.e., there is only one possible value of the random variable which can occur (Figure F-5). The value taken on by the random variable is the mean value, or expected value, and the variance is 0.

This distribution is used to cause total failure of a fraction (0-1) of containers and/or cladding at any time during the simulation. The impact of disruptive events on waste packages is simulated by using this distribution with an adjusted density at the time of the event. The adjusted density reflects the magnitude of the event with respect to container and cladding failure.

References

Benjamin, J.R. and C.A. Cornell, 1970, Probability, Statistics, and Decision for Civil Engineers, McGraw-Hill Book Company, New York.

Hogg, R.V. and A.T. Craig, 1978, Introduction to Mathematical Statistics, 4th Edition, Macmillan Publishing Co., Inc., New York.

FIGURE **F-1**
**EXPONENTIAL PROBABILITY
DENSITY FUNCTIONS**
ARGONNE/MODEL DEVELOPMENT

FIGURE **F-2**
**WEIBULL PROBABILITY
 DENSITY FUNCTIONS**
 ARGONNE/MODEL DEVELOPMENT

FIGURE **F-3**
WEIBULL DISTRIBUTION
PARAMETER WEIGHTINGS
 ARGONNE/MODEL DEVELOPMENT

FIGURE **F-4**
UNIFORM PROBABILITY DENSITY FUNCTION
ARGONNE/3W DEVELOPMENT/WA

FIGURE **F-5**
DEGENERATE PROBABILITY DISTRIBUTION
ARGONNE/3W DEVELOPMENT/WA

APPENDIX G

COMPUTING POISSON TRANSITION RATES FOR PATHWAY FLOW MODES

Chapter 4 of the manual discusses the RIP pathways module. As discussed in Chapter 4, RIP uses a computed breakthrough curve to compute the mass transport rate through a given pathway. The breakthrough curve is a function of pathway length and flow-mode parameters. Each pathway has one or more flow modes. When there are multiple flow modes, RIP uses an approximate Markov-process algorithm to calculate the breakthrough curve. The Markov-process algorithm is a mathematical description of how a particle flowing through a pathway will transition between flow modes. We use Poisson transition rate parameter to describe the likelihood of transitioning between flow modes. Each flow mode of a pathway has its own Poisson transition rate. However, the RIP user specifies a transition rate for only one flow mode. The remaining transition rates are computed using the given transition rate and the flow proportions for the flow modes, f_{Qi} . This appendix presents the solution method that RIP uses to solve for the values of Poisson transition rates in a pathway.

The solution for flow mode transition rates is derived by combining the Markov and Poisson processes. The fundamental principle of the m -state Markov process is that the state probability distribution at time $t + \Delta t$ depends only on the state probability distribution at time t (Cox and Miller, 1965).

In the RIP model, the m -states correspond to the m -flow modes of a pathway. The state probability distributions indicate the likelihood for a particle to be in a particular flow mode during transit along a pathway. The m -state Markov process may be written in terms of matrix and vector quantities as the following:

$$\begin{bmatrix} p_1^{t+\Delta t} \\ p_2^{t+\Delta t} \\ p_3^{t+\Delta t} \\ . \\ . \\ . \end{bmatrix} = \begin{bmatrix} P_{11} & P_{21} & P_{31} & . & . & . \\ P_{12} & P_{22} & P_{32} & . & . & . \\ P_{13} & P_{23} & P_{33} & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{bmatrix} \begin{bmatrix} p_1^t \\ p_2^t \\ p_3^t \\ . \\ . \\ . \end{bmatrix} \quad (G-1)$$

where:

- m is the number of states or flow modes
- $p_i^{(t)}$ is the probability of being in mode i at time t
- $p_i^{(t+\Delta t)}$ is the probability of being in mode i at time $t + \Delta t$
- P_{ij} is the probability of transitioning from mode j to mode i

The elements of the matrix $[P]$ are transition probabilities, indicating the likelihood to transition from one state to another. Thus, element P_{ij} is the probability to go from state j to state i . The elements of the vector $p^{(t)}$ are the probabilities for a given nuclide to be in each of the m modes.

Thus, vector element p_j is the probability to be in mode j . Consequently, the product of $P_{ij}p_j^{(t)}$ is the probability to go from mode j to mode i at time $t + \Delta t$.

The vectors and matrix of Equation G-1 can be represented using an abbreviated notation as follows:

$$p^{(t+\Delta t)} = [P] p^{(t)} \quad (G-2)$$

where:

$p^{(t)}$ is the probability-state vector at time t

$p^{(t+\Delta t)}$ is the probability-state vector at time $t + \Delta t$

$[P]$ is the probability of transitioning from mode j to mode i

As t approaches infinity, the state probability distribution approaches an equilibrium probability distribution, thus, in Eq. 1, $p^{(t)} = p^{(t+\Delta t)}$ as t approaches infinity. For large values of t , Eq. G-2 may be written as:

$$p = [P] p \quad (G-3)$$

where p is the equilibrium state probability distribution vector.

The Poisson probability distribution describes the likelihood for an event to occur given an occurrence rate for the event (e.g. Hogg and Craig, 1978). We can use the Poisson distribution to determine the probability that a particle transitions between flow modes given the transition rate, r , for the particle. The probability that 0 transitions occur in a length dl is:

$$P(N = 0) = 1 - r dl - o(dl) \quad (G-4)$$

The probability that 1 transition occurs in a length dl is:

$$P(N = 1) = r dl + o(dl) \quad (G-5)$$

where:

N is the number of transitions occurring in dl ,

dl is the length interval,

r is the Poisson transition rate, and

$o(dl)$ is a function such that as $dl \rightarrow 0$, $o(dl)/dl \rightarrow 0$, and $o(dl) + o(dl) = o(dl)$.

The diagonal terms of the transition probability matrix $[P]$ may be equated to the probability for 0 transitions ($1 - r dl - o(dl)$) on an interval dl , as they are the transition probabilities to go from state i to state i , i.e., the probability not to transition from the current state.

In the matrix $[P]$, the remaining off-diagonal transition probabilities are unknown, thus, the linear system in Equation G-3 has far more unknowns than knowns and cannot be used to obtain a meaningful solution for the Poisson transition rates. In order to solve for the Poisson transition rates, we make an assumption which results in the transition probabilities of $[P]$ becoming functions of the transition rates, r_i . Our assumption is that the transition probabilities represent the intersection of two independent events. One event is that a particle leaves the current state, and has probability $rdl + o(dl)$. The other event is that the particle enters a new state, conditional on not remaining in the current state. This latter event has probability $p_i/(1-p_j)$ for a particle leaving mode j and entering mode i . Recall the probability, p_i , is the proportion of flow occurring in state i , i.e., $f_{Qi} = p_i$. The off-diagonal transition probabilities of $[P]$ are given by the product of the two event probabilities as follows:

$$P_{ij} = \frac{P_i}{1 - P_j} [r_j dl + o(dl)] \quad (G-6)$$

Equation G-3 may now be solved for the Poisson transition rates as follows:

- Step 1: Note that $[P] = [I] + dl[T]$ where $[I]$ is the m -by- m identity matrix and $[T]$ is a new matrix with diagonal terms equal to $-r_i - o(dl)/dl$ and off diagonal terms equal to $p_i/(1-p_j)(r_j + o(dl)/dl)$; dl is a scalar;
- Step 2: Substitute the results of step 1 into Equation G-3 to obtain the linear system $[T]p = 0$;
- Step 3: Take the limit as $dl \rightarrow 0$ of $[T]$, which results in all terms $o(dl)/dl \rightarrow 0$
- Step 4: by inspection rewrite $[T]p = 0$ such that $[T^*]r = 0$ where r is the vector of transition rates and $[T^*]$ is a new matrix. The diagonal terms of $[T^*]$ are equal to $-p_i$ and the off-diagonal terms are equal to $P_i P_j / (1 - p_j)$.

The linear system given by $[T^*]r = 0$ has an infinite number of possible solutions (i.e., in reduced row echelon form, the last row of $[T^*]r = 0$ contains all zeros). If one value of r is specified, say r_k , the linear system may be solved uniquely for the remaining r_i . This linear system may be written as $[A]x = b$ where the terms in b are equal to $-r_k p_i p_k / (1 - p_k)$ and $[A]$ is an $(m-1)$ by $(m-1)$ matrix. The coefficients of $[A]$ are identical to $[T^*]$, although, the k th row and column from $[T^*]$ is not included in A . In the RIP model, the solution to this system is computed by performing LU decomposition of $[A]$, and then solving for r by back-substitution.

APPENDIX H

ERROR ANALYSIS OF APPROXIMATE MARKOV PROCESS ALGORITHM

The RIP program uses an approximate Markov process algorithm to compute breakthrough curves for the pathways model, as discussed in detail in Section 4.3. This appendix presents an error analysis to compare the approximate Markov process algorithm to the true solution computed using a full Markov random simulation. Comparison between the approximate and true solution was based on particle tracking over the full length of the pathway.

A total of 10 tests were run for a unit-length pathway to compare the approximate Markov process algorithm to the true solution obtained by random simulation. The tests were set up to be generally similar to the anticipated data sets for the RIP model. The tests were different from one another in their flow distributions and flow mode transition rates. In general, while holding the flow distribution constant, tests were run at low, intermediate, and high transition rates. The distance traveled by a typical particle before moving to a different flow mode is proportional to the inverse of the transition rate. For the unit length pathway used in these tests, the low transition rates were on the order of 10^{-2} m^{-1} . This corresponds to a typical distance within a single pathway of the order of 100m. The intermediate transition rates were on the order of 10^{-1} m^{-1} . The high transition rates were on the order of 10^1 m^{-1} . Three to four variations in the flow distributions were used in the tests.

The test results are shown on Figures H-1 through H-10. Tests 1 through 3 are examples of a two-flow mode pathway. One of the flow modes has a high velocity (1 m/yr) and a low proportion of the flow (0.1). The other mode has substantially lower velocity (10^{-4} m/yr) and the majority of the flow (0.9). This pathway may be representative of an unsaturated groundwater system. In this conceptual model the unsaturated matrix has negative pore pressure, drawing water in the fractures into the matrix. The transition rates in tests 1, 2, and 3 were low, intermediate, and high, respectively. The results show that for low transition rates the approximation matches the true solution very well. However, as the transition rates increase, the approximation tends to overestimate the travel time. The largest overestimation is about 1.5 times greater than the true solution. As discussed in Chapter 4, the significance of this error depends on the amount of uncertainty in the flow mode parameters.

The next sequence of tests, 4, 5, and 6, are basically identical to tests 1, 2, and 3, except the flow distribution was changed from (0.1, 0.9) to (0.5, 0.5). The results for these tests are shown on Figures H-4, H-5, and H-6. The results follow a similar pattern to those of the first three tests. In test 6, however, the late travel times are underestimated by the approximation, rather than overestimated. The true solution shows greater dispersion than the approximation. Again, the margin of error is relatively small.

In tests 7, 8, and 9, a two-flow mode system is again used for the comparison. The velocities have not been changed, however, the high velocity flow mode receives the majority of the flow (0.9). This flow distribution may be representative of a saturated groundwater system in fractured rock. In this conceptual model, although the matrix may contain the majority of the water, most of the flow is through the fracture system. The tests include results for low, intermediate, and high transition rates, which are shown on Figures H-7 through H-9. The results show that under low transition rates little error occurs. At greater transition rates, however, the error increases and the approximate method tends to underestimate travel time at the intermediate transition rates. At the high transition rate, the approximate solution compares

well to the true solution, although it contains less dispersion in the travel time distribution causing error to occur for the later travel times. Again, this error is within a factor about 1.5 of the true solution.

Test 10 includes 5 flow modes with a flow velocity variation on the order of 10^4 . The results of test 10 are shown on Figure H-10. The flow is distributed to the flow modes in approximately equal portions. The transition rates are at the intermediate level relative to the previous tests. The test results show that in the region of intermediate travel times, i.e., 10 to 1500 years, the approximation overestimates the true solution. After about 1500 years, the approximation underestimates the true solution. In general, a close match is only achieved for the very early and late travel times over the pathway.

2 - Flow Modes
 Flow Proportions:
 0.1, 0.9
 Flow Velocities:
 1.0, 10^{-4}
 Transition Rates:
 10^{-2} , 10^{-3}

FIGURE **H-1**
TEST 1 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
 ARGONNE/MODEL DEVELOPMENT

2 - Flow Modes

Flow Proportions:
0.1, 0.9

Flow Velocities:
1.0, 10^{-4}

Transition Rates:
1.0, 10^{-1}

FIGURE **H-2**
TEST 2 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
 ARGONNE/MODEL DEVELOPMENT

FIGURE **H-3**
TEST 3 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
 ARGONNE/MODEL DEVELOPMENT

2 - Flow Modes

Flow Proportions:
0.5, 0.5

Flow Velocities:
1.0, 10⁻⁴

Transition Rates:
10⁻², 10⁻²

FIGURE **H-4**
TEST 4 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
ARGONNE/MODEL DEVELOPMENT

2 - Flow Modes
 Flow Proportions:
 0.5, 0.5
 Flow Velocities:
 1.0, 10^{-4}
 Transition Rates:
 1.0, 1.0

FIGURE **H-5**
TEST 5 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
 ARGONNE/MODEL DEVELOPMENT

FIGURE **H-6**
TEST 6 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
 ARGONNE/MODEL DEVELOPMENT

2 - Flow Modes
 Flow Proportions:
 0.9, 0.1
 Flow Velocities:
 1.0, 10⁻⁴
 Transition Rates:
 0.01, 0.09

FIGURE **H-7**
TEST 7 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
 ARGONNE/MODEL DEVELOPMENT

2 - Flow Modes

Flow Proportions:
0.9, 0.1

Flow Velocities:
1.0, 10^{-4}

Transition Rates:
1.0, 9.0

FIGURE **H-8**
TEST 8 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
 ARGONNE/MODEL DEVELOPMENT

FIGURE **H-9**
TEST 9 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
 ARGONNE/MODEL DEVELOPMENT

5 - Flow Modes

Flow Proportions:
0.1, 0.2, 0.3, 0.25, 0.1

Flow Velocities:
 $1.0, 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}$

Transition Rates:
1.0, 0.89, 0.78, 0.83, 0.94

FIGURE **H-10**
TEST 10 - APPROXIMATE MARKOV
PROCESS ALGORITHM ERROR ANALYSIS
ARGONNE/MODEL DEVELOPMENT

APPENDIX I

COMPUTING A RETARDATION PARAMETER FOR MULTIPLE RETARDATION MECHANISM

This appendix presents the calculation method used to combine retardation parameters for use in the RIP algorithm. Retardation parameters are used to adjust flow mode travel times for individual radionuclides. Chapter 4 of the report discusses pathway flow modes and radionuclide retardation.

The retardation parameter based on the advection-dispersion equation for solution transport in porous media is given by the following:

$$R = 1 + \frac{M_s}{M_d} \quad (I-1)$$

where:

R is the total retardation parameter,

M_s is the total sorbed mass, and

M_d is the total dissolved mass.

For more than one retardation mechanism, the quantity of sorbed mass for the i th mechanism is given by the following:

$$M_{s_i} = M_d (R_i - 1) \quad (I-2)$$

where:

M_{s_i} is the sorbed mass resulting from the i th retardation mechanism,

R_i is the retardation parameter for the i th mechanism, and

M_d is the total dissolved mass.

The total sorbed mass is the sum of all sorbed mass given by Eq. I-2, and is given by the following:

$$M_s = M_d \sum (R_i - 1) \quad (I-3)$$

where the parameters are as defined in Eq. I-1 and Eq. I-2. The total retardation parameter representing all retardation mechanisms is obtained by substitution of I-3 into I-1 and is given by:

$$R = 1 + \sum (R_i - 1) \quad (I-4)$$

APPENDIX J

DERIVING DOSE CONVERSION FACTORS

As described in Chapter 6, the computational algorithm for computing doses within RIP is fairly straightforward. The major input parameters are dose factors, which convert concentrations in some environmental media to dose. Deriving dose factors for use in the analysis is the most complex task in dose/risk modeling. Table J-1 gives an example of a dose conversion table. The sections that follow provide an illustration of how a table such as this can be developed.

It should be noted that there is not a unique correct way to calculate a dose factor. The following example illustrates *one* way that dose factors can be computed, and should not be taken to be a *recommended* method of calculating a dose factor. Rather, the following example is provided purely as a basis of discussion to introduce the user to some of the concepts involved.

J.1 General Form

The dose factor from exposure to a concentration of a radionuclide through an environmental pathway is the result of the sum of various sources of exposure. For example, if the pathway is ground water, dose results from direct exposure to the ground water, and the ingestion of food products that have been exposed in some way to the ground water. Direct exposure could include ingestion (drinking) of the water, and immersion (bathing, showering) in the water. Plants irrigated with the water would also contain radionuclides. Livestock could ingest radionuclides from the water by either drinking the water directly, or by ingesting plants irrigated with the ground water.

Dose is a function of the concentration of a radionuclide in the source, the amount of exposure (e.g. number of kilograms ingested, number of hours immersed), the activity of the radionuclide, and the equivalent dose per unit activity of the specific means of exposure. The following equation presents these concepts in a simplified form:

$$D_{rjg} = \sum_a C_{raj} \cdot Q_{ag} \cdot E_r \cdot A_r \quad + \quad [\text{dose from animal products}]$$

$$\sum_p C_{rpj} \cdot Q_{pg} \cdot E_r \cdot A_r \quad + \quad [\text{dose from plant products}]$$

$$\sum_e C_{rj} \cdot Q_{ejg} \cdot E_{er} \cdot A_r \quad [\text{direct dose from pathways}]$$

where:

- C_{rj} = The concentration of radionuclide r in pathway j (g/m^3 or g/kg).
- C_{raj} = the concentration of radionuclide r in animal product a due to radionuclides present in pathway j (g/m^3 or g/kg).
- Q_{ag} = the quantity of animal product a that is consumed by an individual in receptor group g (m^3/yr or kg/yr).

E_r	=	the equivalent dose per activity for ingestion of radionuclide r (Sv/Bq or Sv/Ci; note: $1 \text{ Ci} = 2.7 \times 10^{11} \text{ Bq}$)
A_r	=	the specific activity of radionuclide r (Ci/g or Bq/g)
C_{rpj}	=	the concentration of radionuclide r in plant product p due to radionuclides present in pathway j (g/m ³ or g/kg).
Q_{pg}	=	the quantity of plant product p that is consumed by an individual in receptor group g (m ³ /yr or kg/yr).
Q_{ejg}	=	the amount of exposure to an individual in receptor group g from pathway j via exposure mode (i.e. inhalation, ingestion, contact) e (m ³ /yr, kg/yr, hr/yr).
E_{er}	=	the equivalent dose per activity for ingestion of radionuclide r via exposure mode e (Sv/Bq or Sv/Ci)

Table J-2 provides some example consumption rates (Q_a , Q_p , Q_e) for a hypothetical receptor.

Equivalent dose/activity is a means of accounting for the fact that ingestion of the same amount of activity of two different radionuclides may be different due to the type of particles emitted during radioactive decay, and also provides a means of normalizing the health effects of different means of exposure (e.g. contact and ingestion) to similar amounts of a single radionuclide. Table J-3 provides some examples of activity values and equivalent dose/activity values. (Note: $1 \text{ Ci} = 3.7 \times 10^{10} \text{ Bq}$). Sources for dose/activity values include Schleien et al (1986) and Eckerman et al (1988).

The following sections provide more detail on dose due to ingestion of plant and animal products.

J.2 Radionuclide Concentrations in Animal Products

The concentration of radionuclides in animal products (dairy products and various meats) is a function of the exposure of the source animal to radionuclides, and how the animal absorbs radionuclides. For example, not all radioactive matter ingested by an animal is absorbed into its flesh or milk, some of it is passed through as waste. In addition, absorbed radionuclides tend to concentrate in specific portions of the body, particularly the liver. Concentration of a radionuclide in a particular animal product can be described mathematically as follows:

$$C_{raj} = \sum_p C_{rpj} \cdot Q_p \cdot E_r \cdot A_r \cdot F_{ar} + \quad \text{[from plant products]}$$

$$\sum_e C_{rj} \cdot Q_{ej} \cdot E_{er} \cdot A_r \cdot F_{ar} \quad \text{[from pathways]}$$

where:

F_{ar} = the normalized retention or concentration factor for animal product a due to ingestion of radionuclide r ($[g/kg]/[g/kg]$, or for dairy products $[g/l]/[g/kg]$)

To illustrate how an animal may be exposed to radionuclides, Table J-4 provides some examples of consumption rates for several types of livestock.

Retention factors relate the concentration of radionuclides in an animal product to the daily ingestion rate of the radionuclide by the source animal. Retention factors are radionuclide-specific, and take into account the capacity of different animal to absorb different amounts of various radionuclides. Retention factor values are available from various published sources including Balkema (1983-1985), Ng (1982), Ng et al (1982), Till and Moore (1988), and NSS (1989). Some example values for retention factors are shown in Table J-5.

J.3 Radionuclide Concentrations in Plant Products

The concentration of radionuclides in plant products (terrestrial and marine) is a function of the exposure of the plant to radionuclides in its nutrient sources (i.e. water, soil and air) as follows:

$$C_{rpj} = \sum_e C_{rj} \cdot Q_{ej} \cdot E_{er} \cdot A_r \cdot F_{pr} \quad [\text{dose from pathways}]$$

where:

F_{pr} = the normalized concentration factor for plant product p due to consumption of radionuclide r

Concentration factors are plant equivalent to retention factors. Concentration factor values are available from various published sources including Balkema (1983-1985), NSS (1989), Ng (1982), Ng et al (1982), Till and Moore (1988). Some example values for retention factors are shown in Table J-5.

J.4 References

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TABLE J-1
Computed Dose Factors

Radio-nuclide	soil (mSv/yr)/ (g/kg)	well (mSv/yr)/ (g/m ³)	river (mSv/yr)/ (g/m ³)	surface water (mSv/yr)/ (g/m ³)	ocean (mSv/yr)/ (g/m ³)	atmosphere (mSv/yr)/(g/m ³)
AC227	3.13e+07	6.10e+09	6.38e+06	6.38e+06	1.22e+09	8.18e+12
AM241	2.80e+05	4.54e+07	3.99e+04	3.99e+04	7.95e+07	1.59e+11
AM242		7.34e+04				5.11e+07
AM243	1.26e+04	2.62e+06	2.31e+03	2.31e+03	4.60e+06	9.27e+09
CA41	1.44e+02	4.76e+02	3.26e+00	3.26e+00	6.95e-01	7.43e+03
CO60	6.20e+07	1.83e+08	2.12e+06	2.12e+06	2.89e+08	2.18e+10
CS135	9.48e+00	4.88e+01	8.15e+00	8.15e+00	2.11e+00	4.81e+02
CS137	5.08e+06	2.61e+07	4.36e+06	4.36e+06	1.13e+06	2.56e+08
H3	2.35e+06	3.64e+06	1.23e+05	1.23e+05	1.99e+06	5.49e+07
I129	6.96e+01	2.93e+02	4.90e+00	4.90e+00	1.92e+01	2.71e+03
N159	6.54e+00	9.37e+01	3.25e-01	3.25e-01	6.27e+01	1.80e+04
NP237	2.15e+02	1.68e+05	1.40e+02	1.40e+02	6.22e+03	3.09e+07
PA231	6.69e+04	3.00e+06	3.01e+03	3.01e+03	1.66e+05	3.55e+09
PB210	4.65e+08	2.46e+09	1.68e+08	1.68e+08	6.28e+08	6.19e+10
PU238	2.06e+05	4.06e+07	3.57e+04	3.57e+04	1.37e+07	4.71e+11
PU239	8.00e+02	1.64e+05	1.45e+02	1.45e+02	5.54e+04	1.85e+09
PU241	2.55e+04	5.40e+06	4.74e+03	4.74e+03	1.82e+06	5.21e+10
PU242	4.67e+01	9.58e+03	8.43e+00	8.43e+00	3.23e+03	1.08e+08
RA228	7.61e+07	2.35e+09	5.72e+06	5.72e+06	6.01e+08	1.14e+11
SE79	5.55e+03	3.68e+03	1.62e+02	1.62e+02	1.06e+04	1.01e+05
SN126	1.86e+03	3.32e+03	1.11e+02	1.11e+02	8.49e+04	2.48e+05
SR90	2.12e+08	1.17e+08	9.31e+04	9.31e+04	1.42e+05	1.56e+10
TC99	2.76e+03	1.49e+02	9.62e-02	9.62e-02	2.88e+01	1.24e+04
TH228	1.27e+06	1.95e+09	6.50e+06	6.50e+06	6.87e+08	2.45e+13
TH232	1.22e-03	1.80e+00	6.01e-03	6.01e-03	6.36e-01	1.11e+04
U233	2.69e+01	1.68e+04	2.32e+00	2.32e+00	1.49e+02	1.15e+08
U234	2.34e+01	1.06e+04	1.51e+00	1.41e+00	9.46e+01	7.26e+07
U235	2.31e-01	3.45e+00	4.88e-04	4.88e-04	3.24e-02	2.32e+04
U236	2.27e-01	1.04e+02	1.48e-02	1.48e-02	9.28e-01	7.12e+05
U238	8.11e-03	3.76e+00	5.31e-04	5.31e-04	3.34e-02	2.55e+04

TABLE J-2
Receptor Consumption Rates

TYPE	RATE	UNITS
Dairy	300	l/yr
Beef	60	kg/yr
Beef Liver	20	kg/yr
Beef Kidney	2	kg/yr
Mutton	30	kg/yr
Mutton Liver	20	kg/yr
Mutton Kidney	5	kg/yr
Chickens	10	kg/yr
Eggs	2	kg/yr
Other Animal Products	1	kg/yr
Green Vegetables	80	kg/yr
Root Vegetables	120	kg/yr
Grains	130	kg/yr
Marine Fish	219	kg/yr
Fresh Water Fish	20	kg/yr
Ground Water Well (Drinking)	600	l/yr
Ground Water Well (Immersion)	100	hr/yr
Ocean (Immersion)	10	hr/yr
Soil (Contact)	300	hr/yr
Atmosphere (Inhalation)	8760	m ³ /yr
Atmosphere (Immersion)	8760	hr/yr

TABLE J-3
Equivalent Dose / Activity

Radionuclide	Inhalation (Sv/Bq)	Ingestion (Sv/Bq)	Air Immersion (Sv/y)/(Bq/cc)	Ground Exposure (Sv/y)/(Bq/cm ²)	Activity/Mass (Ci/gram)
AC227	1.81e-03	3.80e-06			7.23e+01
AM241	1.20e-04	9.84e-07	2.30e-02	7.26e-06	3.44e+00
AM242	1.58e-08	3.81e-10			9.73e+00
AM243	1.19e-04	9.79e-07			2.00e-01
CA41	3.64e-10	3.44e-10			6.23e-02
CO60	5.91e-08	7.28e-09			1.13e+03
CS135	1.23e-09	1.91e-09			1.15e-03
CS137	8.63e-09	1.35e-08			8.71e+01
H3	1.73e-11	1.73e-11			9.65e+03
I129	4.69e-08	7.46e-08	1.00e-02	5.50e-06	1.77e-04
NI59	7.31e-10	5.67e-11			7.58e-02
NP237	1.46e-04	1.20e-06			7.06e-04
PA231	3.47e-04	2.86e-06			4.72e-02
PB210	3.67e-06	1.45e-06	1.60e-03	6.90e-07	7.64e+01
PU238	1.06e-04	8.65e-07	1.10e-04	2.10e-07	1.71e+01
PU239	1.16e-04	9.56e-07			6.22e-02
PU241	2.23e-06	1.85e-09			1.03e+02
PU242	1.11e-04	9.08e-07			3.82e-03
RA228	1.29e-06	3.88e-07			2.73e+02
SE79	2.66e-09	2.35e-09			6.98e-02
SN126	2.69e-08	5.27e-09			2.84e-02
SR90	3.51e-07	3.85e-08			1.37e+02
TC99	2.25e-09	3.95e-10	6.30e-07	1.50e-10	1.70e-02
TH228	9.23e-05	1.07e-07			8.20e+02
TH232	4.43e-04	7.38e-07			1.10e-07
U233	3.66e-05	7.81e-08			9.69e-03
U234	3.58e-05	7.66e-08	1.80e-04	1.90e-07	6.26e-03
U235	3.32e-05	7.19e-08	1.90e-01	4.10e-05	2.16e-06
U236	3.39e-05	7.26e-08	1.40e-04	1.70e-07	6.48e-05
U238	3.20e-05	6.88e-08	1.20e-04	1.50e-07	3.37e-07
ZR93	8.67e-08	4.48e-10			2.51e-03

TABLE J-4
Consumption Rates For Livestock

Material	UNITS	Cattle	Sheep	Chicken	Other Animal Products
Pasture (ingestion)	kg/day	20	10	1	1
Soil (ingestion)	kg/day	1	1	0.1	1
Ground Water Well (ingestion)	m3/day	0.01	0.01	0.0001	0.01
River Water (ingestion)	m3/day	0.01	0.01	0.0001	0.01
Surface Water (ingestion)	m3/day	0.01	0.01	0.0001	0.01
Atmosphere (inhalation)	m3/day	10	10	0.1	10
Note: Concentration factors are specified for pasture ingestion (based on assumed rates).					
Estimated consumption rates are used to approximate concentration factors for ingestion of other media.					

TABLE J-5
Normalized Retention and Concentration Factors for AC227

Material	Pasture (g/kg)/ (kg/day)	Soil (g/kg)/ (kg/day)	Well (g/kg)/ (m ³ /day)	River (g/kg)/ (m ³ /day)	Surface Water (g/kg)/ (m ³ /day)	Ocean (g/kg)/ (m ³ /day)	Atmosphere (g/kg)/ (m ³ /day)
Pasture		6.00e-04					
Dairy ¹	1.00e-05	1.00e-05	1.00e-07	1.00e-07	1.00e-07		1.00e-04
Beef	5.26e-05	5.26e-05	5.26e-07	5.26e-07	5.26e-07		5.26e-04
Beef Liver	4.21e-02	4.21e-02	4.21e-04	4.21e-04	4.21e-04		4.21e-01
Beef Kidney	5.26e-05	5.26e-05	5.26e-07	5.26e-07	5.26e-07		5.26e-04
Mutton	2.64e-04	2.64e-04	2.64e-06	2.64e-06	2.64e-06		2.64e-03
Mutton Liver	9.45e-02	9.45e-02	9.45e-04	9.45e-04	9.45e-04		9.45e-01
Mutton Kidney	2.64e-04	2.64e-04	2.64e-06	2.64e-06	2.64e-06		2.64e-03
Green Vegetables		1.00e-03					
Root Vegetables		1.00e-03					
Grains		1.00e-03					
Marine Fish						5.00e-02	
Marine Mollusks						1.00e+00	
Marine Crustaceans						1.00e+00	
Marine Algae						1.00e+00	
Fresh Water Fish				3.00e-02	3.00e-02		
Fresh Water Plants				1.00e+01	1.00e+01		
Dose factors	3.80e+01	3.13e+07	6.10e+09	6.38e+06	6.38e+06	1.22e+09	8.18e+12

¹ - Note: Retention factors for dairy products are in units (g/l)/(kg/day) and (g/l)/(m³/day).

**RIP REPOSITORY PERFORMANCE ASSESSMENT
AND STRATEGY EVALUATION MODEL:**

USER'S GUIDE

Version 4.04

Golder Associates Inc.

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1. INTRODUCTION

This document is a user's guide for the integrated repository performance assessment and strategy evaluation software RIP (Repository Integration Program) developed by Golder Associates Inc. (GAI). The underlying theory and capabilities of the software are described in detail in a companion document. This companion document, the RIP Theory and Capabilities Manual, *should be read prior to using this user's guide* and is *required reading* to ensure appropriate application of the RIP software.

The purpose of this document is to provide the specific information required to specify input and use the RIP program. This document discusses hardware requirements, the basic structure of the software, data entry and application of the model, and post-processing of results. In combination with the RIP Theory and Capabilities Manual, this document provides the necessary documentation and instructions to use the RIP software.

Chapter 2 describes the basic RIP model philosophy and structure, including a summary of RIP theory and capabilities, a discussion of the philosophy, structure and flexibility of the user interface, and details of hardware requirements and software installation. Chapter 3 then provides an overview of the RIP user interface, describing the menu organization and the basics of data entry and manipulation. Chapter 4 describes the RIP Parameters module, the software component which enables model parameters to be defined by the user stochastically and/or as functions of other parameters. This module is a cornerstone of the RIP methodology and an understanding of its structure and capabilities, and the flexibility that it imparts to the model, is required to fully apply RIP. Chapter 5 then discusses in detail the actual data entry and application of the performance assessment model. Chapter 6 discusses data entry and application of the strategy model. Finally, Chapter 7 describes post-processing of RIP results. References are included in Chapter 8.

2. BASIC RIP MODEL PHILOSOPHY AND STRUCTURE

2.1 Overview of RIP Background and Methodology

2.1.1 The Role of Performance Assessment

Traditionally, performance assessment has been considered as an essential analysis to be implemented at the later stages in a repository program in order to demonstrate that the candidate site is in compliance with the licensing criteria. Performance assessment, however, can also be used as a tool to aid in the development and implementation of the entire siting and design procedure. In fact, Golder Associates and others have long maintained that the only effective way to make valid site selection, characterization and design decisions (what should be studied, when, and in what detail) is by using preliminary iterative total system performance assessments (e.g., Golder Associates, 1977; NRC, 1983; Golder Associates, 1986). This view has been reiterated in the United States by both the National Research Council (1990) and the Nuclear Waste Technical Review Board (1990), and internationally by the NEA (1991).

This view of an ongoing iterative performance assessment-driven design and characterization process is based on the premise that by evaluating system performance using *currently available knowledge and the anticipated level of knowledge that can be obtained following completion of a site selection, characterization, or design activity*, it will be possible to identify which activities will be most critical to rapid and accurate determination of site and design suitability. Figure 2-1 illustrates the intended process graphically.

The RIP methodology has a two-fold purpose:

- to provide a systematic framework for organizing and quantifying the current knowledge (and uncertainty) regarding the performance of the entire repository system; and
- to act as a management tool to aid decision making (e.g., regarding site selection, characterization and design issues) and to help assure continuing program refinement.

The first item listed above has become very apparent to Golder Associates in the process of eliciting information regarding models and input data from scientists and engineers involved in several international repository programs. Namely, the performance assessment model (and the process of eliciting model input) can act as a mechanism and framework for integrating the available information generated by different groups into a meaningful whole (allowing one to keep the "big picture" and the ultimate aims of the project clearly in focus). Such an integration is not only useful for project managers (and is ultimately required in order to carry out a

FIGURE 2-1
METHODOLOGY OVERVIEW
ARGONNE/MODEL DEVELOPMENT

meaningful assessment of site suitability), but can also help individual project scientists and engineers formulate and present the results of their research in a manner such that it can be *readily applied* to the ultimate goal of the project, *predicting the performance and determining the suitability of a selected site*.

The second item means that a tool such as RIP can be used in an ongoing review process to continually re-evaluate which data needs are most critical, and to reallocate program resources appropriately.

2.1.2 Performance Assessment Modeling Approach

In general terms, performance assessments can be broadly divided into two categories: those based on a "top down" approach, and those based on a "bottom up" approach. RIP is based on a "top down" approach.

"Bottom up" approaches to performance assessment attempt from the outset to model the various controlling processes in detail, and typically make use of complex *process-level models* for the various system components. The emphasis is on understanding and explaining the processes in great detail in order to eventually describe the behavior of the entire system. Due to the complexity of real systems, however, properly implementing and integrating the various process-level component models and examining total system behavior *while incorporating uncertainty* can be quite difficult. Moreover, under a "bottom up" approach, a large amount of time and money can be inadvertently spent studying processes and parameters which are of little or no importance to repository performance.

As a result, Golder Associates believes that although detailed process-level modeling is ultimately required for credible performance assessments, this detailed modeling should be organized and structured at a higher level using a "top down" approach.

Rather than starting at the bottom and attempting to simulate the physical processes in great detail, "top down" approaches to performance assessment start from the top and concentrate on the *integration* (at a much higher level) of all system components. The controlling processes may initially be represented by approximate high-level (i.e., less detailed) models and parameters. In general, these high-level parameters will take the form of subjective assessments (of probability distributions) from qualified experts.

There are two key points in the application of a "top down" performance assessment approach:

- 1) Less detailed component models and associated high-level parameters must incorporate an accurate representation of the *model and parameter uncertainty* resulting from the approximations.
- 2) As opposed to representing all processes with great detail from the outset (whether or not it is justified), details are only added when it is warranted (e.g., if additional data is available and results indicate that performance is sensitive to a process which is currently represented in a simplified manner with a correspondingly large degree

of uncertainty). That is, details are only added to those processes which are identified as being important with respect to system performance.

As mentioned above, in a "top down" approach, each system component may initially be represented at a relatively high level. The total system model can then evolve by adding detail (and reducing uncertainty) for specific components as further information becomes available. Such an approach can help to keep a project focused on total system performance without getting lost in what may prove to be unnecessary details.

It is important to understand that a "top down" model does not have to be "simple". Whereas a "simple" model might completely *ignore* a key process, a well designed "top down" model *approximates* the process while explicitly incorporating (using probability distributions) the resulting uncertainty which is introduced.

Although detailed process-level models may not be directly implemented when using such a "top down" approach, this is not to say that detailed modeling is not required. Quite to the contrary, detailed process-models form the foundation for a "top down" total system model such as RIP and are required in order to generate the appropriate input parameters for the top-level model. These input parameters may be in the form of analytical expressions or response surfaces developed by an expert based on detailed modeling results. That is, in formulating the high-level input, the expert will typically base his or her opinion as to the value and the associated uncertainty of a parameter or model on available detailed process-model (or experimental) results.

Figure 2-2 schematically presents the information flow within a "top down" performance assessment approach. Note that information must flow in both directions. At the base of the system are process-level models and field and laboratory experiments. This information is then assimilated by experts into a form that can be used in a total system model. The downward flow of information from the total system model consists of identification of the processes and parameters to which system performance is sensitive and a request for further information.

2.1.3 Terminology

The experienced reader will note that the term "model" is used somewhat loosely in this report. Because modeling and simulation terminology is generally not used uniformly throughout the engineering and scientific community, it is important to clearly define at the outset our set of terminology. In particular, it is important to differentiate between what we refer to as the *computational model*, the *conceptual model*, and the *simulation model*.

FIGURE 2-2
TOP-DOWN PERFORMANCE
ASSESSMENT INFORMATION FLOW
ARGONNE/MODEL DEVELOPMENT

As used here, the computational model is the tool which provides the mathematical and computational framework for modeling a system of processes. It is more accurately referred to as the *computational algorithm* or *simulator*. It does not specifically describe an actual physical system. Rather, it consists of a set of flexible tools (i.e., a group of algorithms) for doing so. The computational model is embodied within software (i.e., a computer code). The user of the software must provide the proper input data in order to simulate an actual physical system.

A *conceptual model* is a representation of the physical and chemical properties and processes controlling behavior of a physical system. That is, a conceptual model is essentially a body of ideas, based on available data, which summarizes the current understanding of a system. The conceptual model not only includes a description and quantification of the controlling processes and parameters, but also quantifies the uncertainties involved. (In fact, due to large uncertainties involved in geological systems, a number of alternative conceptual models are likely to be developed.)

The simulation model is the actual implementation of the computational model for a given conceptual model. That is, the simulation model couples the tools within the computational model (the actual computer code) with a particular conceptual model (represented by a distinct set of input data for the computer code).

Summarizing in general terms, the *computational model* is the mathematical framework embodied in the actual computer code. A *conceptual model* represents the current understanding of the physical system to be modeled. A *simulation model* is the application of the computer code using a specific data set in order to simulate the behavior of the system described by the conceptual model.

In this document, the term "model" used by itself refers only to the *computational model*. Hence, when we speak of the "radionuclide transport component model" or the "waste package component model", we are referring to the computational algorithms describing radionuclide transport pathways or waste package behavior, respectively (a component model being a subset or part of the total computational model). The complete terms "*conceptual model*" and "*simulation model*", on the other hand, are always used explicitly when referring to these two concepts.

2.1.4 Total System Performance Assessment Model

The major portion of the RIP software is the *total system performance assessment (PA) model*. The PA model is essentially a radionuclide transport model which consists of a series of interconnected, fully-coupled component models. The component models consist, in general, of simplified functions relating various system parameters that control processes affecting radionuclide transport. The primary component models address: 1) waste package behavior and radionuclide release, and 2) transport pathways to the accessible environment. Additional component models describe disruptive events (such as human intrusion, tectonics and volcanism), and fate and effect (dose/risk) of radionuclides in the biosphere. Figure 2-3 is a schematic of the structure of the performance assessment model.

RIP is *not* a detailed deterministic model based completely on low-level physically-based parameters. (For example, it does not explicitly model radionuclide transport through the unsaturated and saturated zone by solving a three-dimensional advection-diffusion equation.) RIP is a *probabilistic model* that is intended to directly represent the uncertainties in processes and events and their controlling parameters. RIP is intended to describe, rather than explain system behavior. Hence, RIP is based on higher-level parameters which represent the controlling processes, without necessarily directly simulating the details. This is not to say that detailed models of the controlling processes are ignored. It is intended that such detailed models be used to generate the appropriate input parameters for RIP (e.g., in the form of response surfaces or approximate analytical expressions).

The RIP performance assessment software is similar to a spreadsheet: while it contains a large amount of built-in logic and computational capabilities, the problem that is solved is entirely defined by the user. RIP has been developed such that it is relatively free of assumptions regarding the details of waste package behavior and radionuclide transport processes. That is, the model consists of a basic computational framework representing the controlling processes, but is intentionally flexible such that the user can represent the processes with as much detail as desired.

Due to the inherent uncertainties resulting from our lack of knowledge, many of the parameters that control processes related to the performance of a repository can only be represented by probability distribution functions (pdfs), as opposed to single values. RIP is designed such that uncertainties in both the model parameters *and* the component models themselves can be explicitly represented.

The RIP model uses a *simulation approach*, utilizing the Monte Carlo method to sample the probability distributions for the uncertain parameters (describing both processes and events) and simulate a large number of system realizations in order to determine probability distributions of site performance (e.g., cumulative release, transport time). That is, RIP steps through time and creates a time history of disruptive events and other system parameters for each system realization, simulates the behavior of the system under those conditions, and then combines the results of all of the realizations in an appropriate manner to determine probability distributions of site performance. Because model parameters are described stochastically, each realization produces a different time history of events and processes. The integrated model is designed such that it can handle all combinations of model parameters and time histories that might be realized. RIP utilizes an importance sampling scheme to increase the efficiency of the Monte Carlo sampling process. Figure 2-4 summarizes the performance assessment model simulation logic.

FIGURE **2-3**

RIP PERFORMANCE ASSESSMENT MODEL COMPONENTS
ARGONNE/MODEL DEVELOPMENT

FIGURE 2-4
RIP SIMULATION LOGIC
ARGONNE/MODEL DEVELOPMENT

In general terms, the output for the performance assessment model consists of performance measures for the repository system. These performance measures are probabilistic in nature. That is, output is not a single value, but a distribution that specifies the probability of exceedance for any particular value for the performance measure (e.g., cumulative release to the accessible environment, peak individual dose). Figure 2-5 illustrates three ways in which such results can be presented.

2.1.5 Strategy Evaluation Model

The performance assessment model can be run independently to produce probabilistic measures of performance for a site (e.g., cumulative release to accessible environment, peak individual dose). In addition, however, the PA model can be used as a component of a probabilistic decision analysis strategy assessment model. Conceptually, the strategy model can be thought of as a shell that contains the performance assessment model. That is, the PA model is embedded within a decision analysis model that allows the user to evaluate alternative site characterization strategies.

Figure 2-6 provides a schematic of the RIP strategy evaluation model. The RIP user defines a characterization *strategy*, which consists of a set of characterization or design *activities*. A characterization/design activity is a specific scientific study or group of studies proposed for the site (e.g., surface-based testing). For each activity, the user specifies the estimated cost, the estimated duration (including required precedent activities), and the degree to which the uncertainty in one or more system parameters may be reduced by the activity.

Given a current ("prior") data set of system parameters, RIP uses this information regarding activities to realize a large number of sets of post-strategy system parameter distributions ("posteriors"). That is, the current data set (in particular, the uncertainty in specified system parameters) is modified to reflect the effects of carrying out the activities within a characterization strategy. Because we can not predict precisely how a parameter's distribution will change due to an activity, but can only estimate how the *magnitude of the uncertainty* will be affected (i.e., the distribution shape may narrow, but we can't predict whether it will shift left or right), the results of a particular strategy can only be described probabilistically. In other words, a particular strategy defines a probability distribution of *sets of system parameter distributions*. The RIP strategy model samples this distribution of sets many times.

Based on the parameter distributions within a given realized set, RIP produces a probabilistic evaluation of repository performance measures. Each realized set of parameter distributions produces unique probabilistic performance results (e.g., in the form of a CCDF of dose or cumulative release). Figure 2-7 illustrates this schematically. By realizing many different sets of parameter distributions for a particular strategy, producing a probabilistic performance result for each, and combining this suite of results in an appropriate manner, it is possible to

a) Probability density function

b) Cumulative distribution function

c) Complementary cumulative distribution function

FIGURE **2-5**
PRESENTATION OF
PROBABILISTIC RESULTS
 ARGONNE/MODEL DEVELOPMENT

FIGURE 2-6
OVERVIEW OF RIP
STRATEGY EVALUATION
ARGONNE/MODEL DEVELOPMENT

FIGURE 2-7
**SUITE OF PERFORMANCE
 RESULTS FOR STRATEGY A**
 ARGONNE/MODEL DEVELOPMENT

determine probabilistically how that particular strategy will effect the evaluation of site suitability. Figure 2-8 presents an example of how the results shown in Figure 2-7 can be combined to evaluate the effect of the strategy.

In practice, the algorithm used in RIP is somewhat less complex than that indicated in Figure 2-6. It is not actually necessary to re-run the performance model each time the updated probability distributions are produced by simulating a strategy. In fact, it is only necessary to run one full set of performance model analyses. Subsequently, the relative probabilities of each realization can be modified based on the updated probabilities for the parameters to create the revised performance probability distributions (such as those shown in Figure 2-7).

Both the performance assessment model and the strategy evaluation model are discussed in detail in the RIP Theory and Capabilities document.

2.2 Parameter Definition and the Flexibility of the User Interface

The cornerstone of the RIP methodology, which is critical to understand in order to take full advantage of the software, is the concept that model input parameters can be defined by the user with a great deal of flexibility. In particular, *a given system parameter can be specified as a constant, a stochastic (i.e., represented as a probability distribution), or as a function of other parameters* (which themselves can be constants, stochastics, tables, or functions).

Representing system parameters as *stochastics* allows the RIP user to specify the degree of *uncertainty* in a particular parameter. For example, if the current level of knowledge regarding a particular system parameter (such as an elemental solubility) is such that it is only possible to specify its value within certain limits (e.g., greater than 10^{-4} g/m³ but less than 10^{-1} g/m³), it would be most appropriate to specify this parameter as a probability distribution (e.g., a log-uniform distribution ranging between 10^{-4} and 10^{-1}). RIP allows the user to choose from a wide variety of probability distributions (e.g., normal, log-normal, triangular, beta, gamma, discrete, etc.) for a stochastic parameter. For each Monte Carlo realization of the repository system, all of the stochastic parameters are sampled from their specified distributions.

The ability to represent system parameters as *functions* of other parameters gives the user the ability to readily add detail to any given system parameter or process represented by RIP. The user can even create and specify processes and parameters which are not explicitly incorporated into RIP. In a sense, the RIP program is similar to a spreadsheet: while it contains a large amount of built-in logic and computational capabilities, the problem that is solved is entirely defined by the user. That is, RIP has been developed such that it is relatively free of assumptions regarding the details of waste package behavior and radionuclide transport processes. Similar to a spreadsheet user, the RIP user can define a very simple model, or a very complex one. Hence, RIP consists of a basic computational framework representing the

FIGURE 2-8
PROBABILITY OF POST-STRATEGY
PERFORMANCE RESULTS
ARGONNE/MODEL DEVELOPMENT

controlling processes, but is intentionally flexible such that the user can represent the processes with as much detail as desired. This allows the conceptual model being represented by RIP to be continuously and easily modified as more information becomes available.

The user interface of the software is designed such that the user literally types in the desired function. In addition to standard mathematical operators (e.g., SIN, COS, MAX, ERF, LOG), the user can define functions using relational operators (e.g., >, <, =) and IF, THEN logic. Such flexibility allows the user to easily modify and add detail to the conceptual and computational model *without having to make changes to the software* (i.e., without modifying and compiling the source code).

As an example, suppose that instead of representing an elemental solubility as a stochastic parameter (as illustrated above), the user wished to incorporate a solubility model which explicitly accounted for the effects of temporally or spatially variable chemistry (e.g., pH) conditions. To accomplish this, the user could define a new parameter, called *pH*. This parameter could be defined as a constant, a stochastic, or a function (of other parameters or of time). It could also be assigned a random spatial variability throughout the repository. The elemental solubility could then be described as a function of these parameters.

For example,

$$\text{SOLN} = (A * \text{pH}) + B \quad (2.1)$$

where SOLN is the solubility of element n and A and B are constants or additional user-defined parameters.

For more complex functions, the software is structured such that the user can develop separate coded functions (i.e., separate coded program modules, written in the C programming language) which can then be directly coupled with the main RIP algorithms.

Use of the *Parameters Module*, the software component that implements the concepts described above, is discussed in detail in Chapter 4.

2.3 Software Structure and Hardware Requirements

The RIP software consists of two independent units, referred to here as the *front end* and the *back end*. The front end comprises the user interface, while the back end contains the actual computational algorithms. Technically, the front end and the back end are two separate programs. The basic structure of the software, including all of the files involved, is illustrated in Figure 2-9. The various input/output files are discussed again in Chapter 7.

1. Read and/or create input data set.
2. Create transfer file.
3. Write realized values of stochastic, event and constant parameters.
4. Write calculated values of function, table and coded function parameters.
5. Run back end and produce results.
6. Read results into front end for post-processing. *
7. Post-process results.

* The original input file (.rp) and binary parameters file (.bpf) must be read into the front end with the results files (.btr, .bsr) when post-processing results.

FIGURE **2-9**
RIP FRONT END/BACK END STRUCTURE
 ARGONNE/MODEL DEVELOPMENT/WA

The user defines the problem to be simulated via the window-driven user interface of the front end. The front end then communicates this information to the back end via a *transfer file*. (The transfer file always has the extension ".btf".) The transfer file is read by the back end, which then carries out the actual computations and produces two separate *results files*. (The two results files always have the same name as the .rp file, with the extensions .btr and .bsr, respectively.) The results files are then read by the front end which processes the results, as directed by the user, into a variety of graphical and text formats.

The front end and the back end operate independently and can be implemented on different machines, with the transfer files and the result files being transferred between the machines electronically (e.g., via a network), or manually (e.g., on a magnetic disk). *Note, however, that because the transfer files and result files are in binary format, the RIP front end and back end must be run on the same platform (e.g., DOS, UNIX) to avoid potential data format conflicts.*

The front end is written in Borland Pascal (Version 7.0) and is intended to be run on a personal computer (PC). A PC with an 80286 processor, a math co-processor, and at least 2Mb RAM is required to run the RIP front end.

The back end is written in ANSI standard C. As a result, the back end is very portable and can be run on a variety of computers. At the very least, a PC with an 80286 processor, a math co-processor, and 640Kb RAM is required to run the RIP back end. Although the back end will run on a PC, because of the computationally intensive nature of the program (i.e., use of the Monte Carlo approach), running complex data sets on certain PCs may be unacceptably slow. In these cases, use of a Pentium processor or a workstation is highly recommended.

2.4 Software Installation and Implementation

The RIP front end is a *protected-mode application*, allowing the program to access up to 16Mb of RAM. This is a necessary feature for creating and handling large input data files. To facilitate this, RIP requires a DOS Protected Mode Interface (DPMI) server and protected mode memory manager. Both of these are provided on the distribution disk.

One implication of the use of a protected-mode application is that running the program simultaneously with memory resident programs (such as a screen grabber) may cause memory conflicts. Although there are ways to minimize these problems (by controlling the amount of memory the protected mode memory manager uses), it is good practice to refrain from running memory resident programs while using RIP. Users interested in controlling the memory management directly (using DOS commands prior to running RIP) should consult the Borland Pascal Version 7.0 Language Guide.

The distribution disks include all of the necessary files to run RIP:

RIP.EXE	executable version of RIP front end;
RIP2.EXE	executable version of RIP back end;
RIP.WNS	file containing input screens for RIP front end;
RIP.HLP	file containing HELP screens;
RTM.EXE	Borland run time manager;
32RTM.EXE	32-bit Borland run time manager;
DPMI16BI.OVL	DOS protected mode interface server;
DPMI32VM.OVL	DOS 32-bit protected mode interface server;
EGAVGA.BGI	graphics driver for screen plots;
HPLJ23.BGI	graphics driver for HPGL2 hard copy plots;
CW3211.DLL	Data link library required by the Borland compiler;
CW3215.DLL	Data link library required by the Borland compiler;
DECAY.BAT	Example batch file for running the back-end with pathway decay;
NODECAY.BAT	Example batch file for running the back-end without decay.

Starting and using the front end of RIP is discussed in detail in the following sections. Because the front end comprises the user interface, supporting data input and post processing of results, this User's Guide is, for the most part, a description of the front end. As will be described subsequently, the back end of RIP is invoked using a single command line. As discussed above, the back end automatically reads in the transfer file created by the front end and creates results files. No other user action is required.

It should be noted that the time scales required to run the front end and the back end will typically be quite different. The front end is an interactive program in which the user specifies data (and manipulates results). While definition of a model can involve weeks or months of data review and analysis, and days to enter and verify the input data, creation of the transfer file is relatively rapid (typically minutes on a powerful PC). The back end, however, is the computational engine for RIP. For large complex simulations with complex input and large numbers of realizations, execution of the back end and the creation of results files may take many hours even when run on powerful machines.

2.5 Software Limitations

The accuracy and applicability of RIP is limited by the modeling assumptions inherent in the software. It is incumbent upon the user to read and understand the Theory Manual and User's Guide and determine whether RIP is suitable for a specific application.

RIP also has limits on the number of parameters, transport pathways, etc. that can be included in a model. RIP provides on-screen warning messages if the user attempts to exceed these limits.

2.6 Model Applicability

Before describing RIP in detail, it is useful to briefly mention the applicability of this simulation tool. The original version of RIP was developed for the U.S DOE for application to the potential high-level radioactive waste repository at Yucca Mountain, Nevada. *Its use, however, is not limited to this particular site.* This is because RIP is designed in a very flexible manner. In simple terms, *RIP is a simulation tool designed to probabilistically model the release of radionuclides from buried waste packages and the subsequent transport of those radionuclides through the environment.*

Hence, although a thorough understanding of the theory and capabilities of RIP is required in order to apply it to any site, its flexibility should allow application to a variety of sites. RIP has been applied to both saturated and unsaturated high-level radioactive waste repositories in a number of geological media (e.g., tuff, salt, granite). RIP has also been applied to hazardous waste (as opposed to radioactive waste sites).

2.7 Required User Training and/or Background

To run RIP, users should have a basic knowledge of DOS. To manipulate RIP models and interpret RIP results, users should have (1) a basic understanding of probability theory; (2) a basic understanding of performance assessment; (3) a basic understanding of the physical system(s) being modeled.

2.8 Error Messages and Reporting

The RIP error messaging strategy is to anticipate user errors and interactively direct the user to make input changes without terminating the program. RIP has over 100 on-screen error messages (not listed here) that are primarily related to input errors by the RIP user. The on-screen error messages provide specific direction to the user to make changes to user inputs to correct the error. The user should follow the directions of the on-screen error message.

User-generated errors generally do not result in termination of the program. However, it is not possible to anticipate all user actions and, infrequently, a "fatal error" occurs (i.e. the program is terminated). In the event of a fatal error, RIP provides, on screen, an error code and code address. The user should copy these codes from the screen and report them to Golder Associates using the forms provided in Appendix D.

In addition, as RIP is applied, users may desire features or modifications that will improve the software. Appendix D of this report contains the forms for reporting software problems and/or suggesting modifications.

3. INTRODUCTION TO THE RIP USER INTERFACE

In this chapter, an introduction to the user interface (i.e., the front end) is presented. The organizational structure of the input windows is discussed, and basic instructions for browsing through the windows, entering data, and saving input files (and screens) are described. The on-screen help utility is also described.

Details of the specific input windows are discussed in subsequent chapters.

Although images of the input screens which are discussed are presented in this document as figures, it may be useful to install and run RIP at this point in order to follow along as various features of the user interface are discussed.

3.1 Getting Started

3.1.1 Creating the Species Table

Prior to running RIP for the first time, it is necessary to create a *species table*. The species table specifies the radionuclide species which are to be included in the RIP simulation. The user also specifies the properties of each species, including the decay rate, specific activity, and daughter product (if any).

The species table is an ascii text file that can be created and edited with any text editor. The file consists of a header line which contains the column heading labels, followed by detail lines containing information for each species. There is one detail line per species. Blank lines and comment lines (lines starting with a !) are ignored and can be used freely throughout the file.

The header line *must* precede all detail lines and *must* start with RNID as its first field. (RNID may or may not be preceded by an "!".) The header line must also contain one item for every column of data. Note that a space is a record delimiter. Hence, a heading cannot have embedded blanks. The required and optional column headers are discussed below.

The first column always contains the radionuclide ids. The id is defined with six alphanumeric characters. RIP compares the alphabetical components of each field which precede any numeric characters in order to identify isotopes of the same element.

In addition to the radionuclide id, at least two of the following three data columns (and associated heading labels) must be in the file:

1. DECAY - the decay rate for the species (1/yr)
2. SPECACT - the specific activity for the species (Ci/g)
3. AWT - the atomic weight

If all three columns are present in the file, RIP ensures that the data are consistent to within 1% (since any two of these items defines the third). If an inconsistency of greater than 1% is found, RIP will terminate with an error message. The relationship between the three parameters is given as follows:

$$\text{SPEC ACT (Ci/g)} = \frac{3.58\text{E} + 05}{\left(\frac{\ln(2)}{\text{DECAY}} \right)} (\text{AWT}) \quad (3.1)$$

- The remaining data columns (and associated heading labels) are optional:
 1. DAUGHTER - the RNID of the daughter product or '-' if species has no daughter. Note that if this column is absent, no decay chains are simulated (i.e., all input is assumed to be '-'). If there is a daughter product, then it must be one of the other species in the table. Note that if a daughter is specified which is not present in the species table, RIP will provide a warning message.
 2. GROUP - the chemical element group for the species. Typically, all isotopes of the same element must have the same chemical element group. If different values are listed for the isotopes of the same element, RIP uses the value for the first isotope of the element in the list. Note, however, that the user has the option to allow chemical element groups to vary by among isotopes of the same element (see Section 5.1.2.5.2). If this option is selected, RIP will use the values as specified in the species table.
 3. LIMIT - the 40 CFR 191 regulatory limit. The default value is zero (in which case the species is skipped during the normalization procedure; i.e., it does not contribute to the normalized release).
 4. LINE - the line style for screen plots. Valid entries for this column are SOLID, DOTTED, DASHED, and CENTER. Invalid entries default to an arbitrary style.
 5. COLOR - the line color for screen plots. Valid entries for this column are BLUE, GREEN, CYAN, RED, MAGENTA, BROWN, LIGHTGRAY, DARKGRAY, LIGHTBLUE, LIGHTCYAN, LIGHTRED, LIGHTMAGENTA, YELLOW, and WHITE. Invalid entries default to an arbitrary color.

Note that RIP is not sensitive to the case of the required heading labels listed above (i.e., they do not need to be all upper case letters). Likewise, RIP is not sensitive to the case of the entries for the LINE and COLOR columns.

An example species table file is shown below:

!rnid	decay	limit	specact	awt	daughter	group	line	color
AC227	3.183E-02	0.20	7.23E+01	227	-	1	dotted	blue
AM241	1.603E-03	0.10	3.44E+00	241	NP237	2	center	green
AM242	4.559E-03	0.10	9.73E+00	242	PU238	2	solid	cyan
AM242M	4.559E-03	0.10	9.73E+00	242	PU238	2	dashed	red
AM243	9.389E-05	0.10	2.00E-01	243	PU239	2	dotted	magenta
C14	1.209E-04	0.10	4.46E+00	14	-	1	center	brown
CA41	4.915E-06	0.20	6.23E-02	41	-	1	solid	lightgray
CL36	2.302E-06	0.20	3.30E-02	36	-	1	dashed	darkgray
CM243	2.432E-02	0.10	5.17E+01	243	PU239	1	dotted	lightblue
CM244	3.829E-02	0.20	8.09E+01	244	PU240	1	center	lightred
NP237	3.238E-07	0.10	0.00E+00	237	U233	2	dotted	magenta
PA231	2.115E-05	0.10	0.00E+00	231	AC227	1	center	brown
PB210	3.108E-02	1.00	0.00E+00	210	-	1	solid	white
PD107	1.067E-07	1.00	0.00E+00	107	-	1	dashed	magenta
PU238	7.897E-03	0.10	0.00E+00	238	U234	1	dotted	lightblue
PU239	2.879E-05	0.10	0.00E+00	239	U235	1	center	lightred
PU240	1.060E-04	0.10	0.00E+00	240	U236	2	dotted	lightcyan
PU241	4.812E-02	0.20	0.00E+00	241	AM241	1	dashed	darkgray
PU242	1.791E-06	0.10	0.00E+00	242	U238	1	dotted	lightblue
RA226	4.331E-04	0.10	0.00E+00	226	PB210	1	center	lightred
RA228	1.205E-01	0.20	0.00E+00	228	TH228	1	solid	blue
TH228	3.622E-01	0.20	0.00E+00	228	-	1	dashed	green
U233	4.372E-06	0.10	0.00E+00	233	TH229	1	dotted	cyan
U234	2.834E-06	0.10	0.00E+00	234	TH230	1	dashed	red
U235	9.845E-10	0.10	0.00E+00	235	PA231	1	center	magenta
U236	2.959E-08	0.10	0.00E+00	236	TH232	1	solid	brown
U238	1.551E-10	0.10	0.00E+00	238	U234	1	dashed	yellow

In addition to the columns discussed above, the user can define additional "extra" columns that represent waste package inventory data or dose conversion factors (the headers for these extra columns are user defined). Importing waste package inventory data will be discussed in section 5.1.2.5.1 and importing dose conversion factors will be discussed in section 5.4.2.

As discussed in Section 3.2.5, the species table can be viewed, but not edited, within the user-interface.

3.1.2 Running the RIP Front End

After creating a species table as described above, the front end program can be started by typing "RIP". The following screen will appear:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Available Memory 368708 file date:			

Repository Integration Program
(c) Golder Associates Inc., 1991, 1992, 1993, 1994, 1995.

This software is version 4.04 of RIP. It has been verified under a quality assurance program, but may contain undetected errors. Any user detecting an apparent error should refer to the User's Guide for instructions on error reporting.

Any permission granted for the use of this program includes the explicit condition that all liabilities and responsibilities for any results obtained from its use are exclusively those of the individual user or organization.

No responsibility is assumed or implied for user support.

RIP will then prompt the user for a file name. This refers to the name of a file to which all of the input information will be saved. If the user specifies a file which already exists, RIP will read this file. The user interface can then be used to edit the information contained in the file. The user can read an existing file automatically when starting RIP by directly specifying the filename in the command. For example, "RIP test" or "RIP test.rp" will automatically load the input file "test.rp".

If the user specifies a new file name (i.e., the name of a file which does not currently exist in the directory), RIP will inform the user that file does not exist, giving him/her the choice to specify a different file name or create a new file. All subsequent changes made during that session will be saved to the specified file. If the user specifies the filename without an extension, the extension ".rp" is automatically added. When a new file is being created, RIP will also prompt for the name of the species table to be used.

The RIP executable file need not be present in the directory from which the command is typed, as long as it is present within the DOS path (typing "path" at the DOS prompt will display the path). Regardless of whether RIP is on the path, the user can type the full pathname for the executable (e.g., "c:\programs\rip\rip test").

Note, however, that the input files for the front-end (the *.rp and species table files) must be in the active directory.

After specifying the filename (and the species table for new files), RIP will prompt for any desired changes to the data file description:

```
[ ] Repository Integration Program (Rev. 4.04 )
  General      PA Model      Strategy Model      Results
  Available Memory 4388420      User's Guide Tutorial      file date: 08-14-95 14:33:56
Change the data file description?
User's Guide Tutorial
```

This short description or title is subsequently displayed at the top of the user interface screen, along with the file date (of the last update), and the amount of random access memory (RAM) currently available on the machine.

3.1.3 Saving Input Files

While in the user interface, the user can save the current input file by hitting <Alt>-<S>. (Note, however, that <Alt>-<S> is not functional until a change has been made to the file.) The user is reminded of this and several additional key combinations (which will be discussed subsequently) at the bottom of every input screen. These prompts, reproduced below, are not shown on the screens printed in this manual.

H:Help F:Families G:General P:Parameters R:RNs S:Save

As a safeguard, RIP will warn a user if he/she has made some changes which have not yet been saved, and tries to exit the program. *Regardless of this safeguard, it is good practice to periodically save large input files while editing.*

As will be discussed in Chapter 7, the RIP post-processor requires a consistent set of input and output files. To facilitate this, RIP automatically write-protects the ".rp" file once a transfer file has been created with it to avoid inconsistencies when post-processing results. Hence, if the user attempts to edit and save such a ".rp" file, RIP warns the user before overwriting the file.

3.2 Basics of the User Interface.

3.2.1 Menu Structure

After specifying the name of the data file, the main window will appear on the screen:

```
[ ] Repository Integration Program (Rev. 4.04 )
  General      PA Model      Strategy Model      Results
  Available Memory 4388420      User's Guide Tutorial      file date: 08-14-95 14:33:56
```

The RIP user interface is structured into a *hierarchy of menus* which provide access to a variety of *interactive data input windows*. The overall menu structure is illustrated graphically in Figure 3-1 and in tabular form in Table 3-1.

FIGURE 3-1
RIP MENU STRUCTURE
ARGONNE/MODEL DEVELOPMENT

Table 3-1 RIP Menu Structure

top level menu item
second level menu item
third level menu item
fourth level menu item

[General]

[PA Model]

- [Waste Package]
 - [Near Field Conditions]
 - [Water Contact Modes]
 - [Temperature Conditions]
 - [Other Factors]
 - [Show Groups]
 - [Waste Package Description]
 - [Make WP Transfer File]
- [Pathways]
- [Events]
- [Dose/Risk]
 - [Receptors]
 - [Dose Conversion Tables]
- [Make Transfer File]

[Strategy Model]

[Results]

Within a menu, the user can move between choices using the right and left arrow keys (or, alternatively, <TAB> and <SHIFT>-<TAB>). The user selects a particular choice by moving to the choice and hitting <ENTER>. Upon selection, either a lower level menu or an input window will appear. *The user can move backward through the structure (i.e., from lower level windows or menus to higher levels) by using the <ESC> key.* Hitting <ESC> from the main (highest level) menu exits the program.

The user can also move between menu items with a mouse. Menu items are selected by clicking on the item. Note that when using a mouse, the user can move backward through the menu structure by clicking on the "[■]" symbol in the upper left hand corner of each window. Clicking on this symbol is equivalent to hitting the <ESC> key.

As the following menu items are briefly summarized below, it is recommended that the user browse the user interface to become familiar with the menu and window structure, and the techniques for moving around within the interface.

As illustrated above, the top level menu consists of four choices:

- [General] provides access to an input window for specifying several general inputs pertaining to graphics setup, echoing of input files, specification of the species table, and several global parameters (e.g., the type of Monte Carlo sampling technique to be used).
- [PA Model] provides access to input windows describing the integrated performance assessment model;
- [Strategy Model] provides access to input windows describing the strategy evaluation model;
- [Results] provides access to the post-processor.

These menu options are discussed in somewhat greater detail below.

[General]

Selection of [General] provides access to a single data input window. The [General] data input window is discussed in detail in Section 3.4.

[PA Model]

Selection of [PA Model] provides access to a second-level menu consisting of five choices pertaining to the total system performance assessment model:

- [Waste Package] provides access to input windows pertaining to the waste package behavior and radionuclide release component model;
- [Pathways] provides access to input windows pertaining to the radionuclide transport pathways component model;
- [Events] provides access to input windows pertaining to the disruptive events component model;
- [Dose/Risk] provides access to input windows pertaining to fate and effect (dose/risk) of radionuclides in the biosphere;
- [Make Transfer File] provides access to a window which is used to specify general simulation information and the form of the output, and to actually run the front end program for the performance assessment model and create a transfer file for the back end.

[Pathways], [Events] and [Make Transfer File] provide direct access to data windows. [Waste Package] provides access to a third-level menu which further subdivides waste package input:

- [Near Field Conditions] provides access to windows for specifying the environmental conditions at the repository;
- [Waste Package Description] provides access to windows for describing the waste package failure and radionuclide release mechanisms;
- [Make Transfer File] provides access to a window that is used to specify general simulation information and the form of the output, and to actually run the front end program for the waste package behavior and radionuclide release component of the performance assessment model and create a transfer file for the back end.

[Waste Package Description] and [Make Transfer File] provide direct access to data windows. [Near Field Conditions] provides access to a fourth level menu that further subdivides the near field conditions input: [Water Contact Modes], [Temperature Conditions], [Other Factors] and [Show Groups].

[Dose/Risk] provides access to a third-level menu which further subdivides dose/risk input:

- [Receptors] provides access to windows for specifying the receptor groups for the biosphere model;
- [Dose Conversion Tables] provides access to windows for describing the factors for converting concentration in some environmental media to a dose to a receptor.

The details of the performance assessment model input windows are discussed in Chapter 5.

[Strategy Model]

Selection of [Strategy Model] provides access to windows pertaining to the strategy evaluation model, allowing the user to define activities within a characterization strategy, and plot probability distributions of cost and duration for the specified strategy. The details of the strategy evaluation model input windows are discussed in Chapter 6.

[Results]

Selection of [Results] provides access to windows pertaining to the post-processing of results. The details of the results input windows are discussed in Chapter 7.

3.2.2 Using Data Input Windows

As described above, the menu structure provides access to the data input windows. For example, the following screen shows the data input window displayed by selecting the menu items

[PA Model]

[Waste Package]

[Waste Package Description]:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
Waste Package Database Editor			
ID : SPENT		Package 1 of 2	F1=Prev
DESC: Spend nuclear fuel			F2=Next
Number of Packages : 10000			F3=Add
MTHM per Package : 1			F4=Del
Waste Burnup (MWd/MTHM): 1			F5=Copy
Is mass transfer/bound exposure independent of failure mode? : No			F6=Copy
Mass Transfer			Inventory
Exposure		Plotting Options	
Primary Container Failure Definition		» Rewetting time : 0	
Secondary Container Failure Definition		» Cont. fail time : 0	
Inventory		Plot axes : automatic	
Define Discharge Pathways			
(AE,1.00)			
Output Selections			
Total Discharges : No		Discharges by RN : No	
Total Discharge Histories : No		Discharge Histories by RN : No	

Many windows for RIP (such as the waste package window illustrated above) are used to specify the details pertaining to a particular unit or structure within the model (e.g., a waste package type, a transport pathway, a disruptive event, a radionuclide). The RIP user interface is designed such that any number of different types of a particular unit or structure can be specified. For example, the user may want to define 3 different waste package types, 12 different pathways, or 3 different disruptive events. To accommodate this, those windows pertaining to these kinds of units or structures can have multiple records or *pages*. Within a window, pages can be added, deleted, or browsed using specified function keys (i.e., F1, F2, F3, F4).

For example, in the screen shown above, the unit of interest is the waste package type. This particular screen indicates in the upper right hand corner of the window ("Package 1 of 2") that two waste package types have been defined (each waste package type being represented on a different page of the window). This particular screen shows page 1 of the window. As indicated in the upper right hand corner, the function keys <F1> and <F2> can be used to browse the pages. Hitting <F2> will bring up page 2 of the screen, which defines waste package type 2:

Repository Integration Program (Rev. 4.04)		Results
General	PA Model	Strategy Model
User's Guide Tutorial		
Waste Package Database Editor		
ID : HLDW	Package 2 of 2	F1=Prev
DESC: vitrified waste		F2=Next
		F3=Add
		F4=Del
		F5=Copy
		F6=Copy
		Inventory
Number of Packages : 10000		
MTHM per Package : 1		
Waste Burnup (MWd/MTHM): 1		
Is mass transfer/bound exposure independent of failure mode? : Yes		
Mass Transfer		
Exposure		
Primary Container Failure Definition	» Rewetting time : 0	
Secondary Container Failure Definition	» Cont. fail time : 0	
Inventory	Plot axes : automatic	
Define Discharge Pathways		
(AE,1.00)		
Output Selections		
Total Discharges : No	Discharges by RN : No	
Total Discharge Histories : No	Discharge Histories by RN : No	

Pages can be added or deleted using the <F3> and <F4> keys, respectively.

As will be described in detail in subsequent sections, function keys can also be used for other purposes (e.g., showing lists, calling up graphics). The available function keys and their uses are always shown on the window.

Within an input window, the user can move between input fields using the arrow keys (or <TAB> and <SHIFT>-<TAB>). A mouse can also be used to move around a particular window. Note that the mouse only moves the cursor within an active window, and can not select items in underlying windows.

Moving through an input window places the cursor in one of four types of input fields: a *descriptive field*, a *data field*, an *option field*, or an *access field*.

A descriptive field is used to provide a description or an identification for a particular process, event or item defined by the window. An *alphanumeric name* or *short description* is entered. In a data field, either a *number* or a *parameter name* is entered.

Within a descriptive or data field, the left and right arrow keys, and the <Home> and the <End> keys can be used for movement. The <Ins>, <Delete> and <Backspace> keys can also be used.

Option fields are used when a list of choices are available to the user. When the cursor is moved to an option field, the field will blink on the screen. There are two ways to select a value from an option field. First, the <PgDn> or <PgUp> keys can be used to toggle through a limited number of input options.. Second, hitting <ENTER> while sitting on an option field brings up a pull-down menu listing all of the available options:

Repository Integration Program (Rev. 402E)			
General	PA Model	Strategy Model	Results
<div> <div>Waste Package Database Editor</div> <div> <div>ID : HLDW</div> <div>DESC: Vitrified Waste</div> </div> <div> <div>Number of Packages : 10000</div> <div>MTHM per Package : 1</div> <div>Waste Burnup (MWd/MTHM): 1</div> <div>Is mass transfer/bound exposure independent of failure mode? : ☐ No ☒ Yes</div> <div>Mass Transfer Exposure</div> <div>Primary Container Failure Definition » Rewetting time : 0</div> <div>Secondary Container Failure Definition » Cont. fail time : 0</div> <div>Inventory</div> <div>Define Discharge Pathways (AE,1.00)</div> </div> <div> <div>Plotting Options</div> <div> <div>Rewetting time : 0</div> <div>Cont. fail time : 0</div> <div>Plot axes : automatic</div> </div> </div> </div>			<div> <div>F1=Prev</div> <div>F2=Next</div> <div>F3=Add</div> <div>F4=Del</div> <div>F5=Copy</div> <div>F6=Copy</div> <div>Inventory</div> </div>
<div>Output Selections</div> <div> <div>Total Discharges : No</div> <div>Discharges by RN : No</div> <div>Total Discharge Histories : No</div> <div>Discharge Histories by RN : No</div> </div>			

The user can move through the options using the arrow keys. An option is selected by moving to the desired choice in the menu and hitting <ENTER>. Throughout this text, these two methods will be used interchangeably when describing option fields.

An access field either *provides access* to a pop-up window or causes a particular action to be carried out (e.g., creation of a file).

In the input window illustrated above, the first two data fields ("ID" and "DESC") are descriptive fields. The next several (through "Waste Burnup") are data fields. The next field, which answers a question regarding mass transfer/bound exposure, is an option field. In this particular case, there are only two options, Yes or No. The input fields starting with "Mass Transfer" and ending with "Inventory" are access fields which call up lower level input windows. For example, selecting "Mass Transfer" and hitting <ENTER> brings up the following screen:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
<div> <div>Waste Package Database Editor</div> <div> <div>ID : HLDW</div> <div>DESC: vitrified waste</div> </div> <div> <div>Number of Packages : 10000</div> <div>MT: ☒ MASS TRANSFER</div> <div> <div>Wa Repository Flow Rate (m/yr): FLOW (21.49758)</div> <div>Is Effective Catchment Area (m²): CATCH (0.5)</div> <div>Ma Geometric Factor for Diffusion (m): OMEGA (0.001)</div> <div>Ex Water Volume Contacting Matrix (m³m³m): 0.1 (Constant)</div> <div>Pr Mass of Sorbent (kg): 1.3 (Constant)</div> <div>Se Equilibrium Partition Coefficients</div> </div> </div> </div>			<div> <div>F1=Prev</div> <div>F2=Next</div> <div>F3=Add</div> <div>F4=Del</div> </div>
<div>Define Discharge Pathways (AE,1.00)</div>			
<div>Output Selections</div> <div> <div>Total Discharges : No</div> <div>Discharges by RN : No</div> <div>Total Discharge Histories : No</div> <div>Discharge Histories by RN : No</div> </div>			

Moving to the desired access field and hitting <ENTER> provides access to the lower level input window or carries out the specified action (access fields are selected by double clicking when using a mouse). Use of descriptive fields and option fields is also straightforward. After typing in characters for a descriptive field, or selecting the desired option in an option field using the <PgDn> or <PgUp> toggle, the <ENTER> key enters the data and moves the cursor to the next input field. If no changes have been made, hitting the <ESC> key will close the window. If data has been modified (in any type of field), hitting <ESC> will undo the changes and restore the original information. Hitting <ESC> a second time will close the window.

Data fields represent the major form of data input. There are actually two types of data fields: *constant data fields* and *parameter data fields*. Constant data fields (which are green on a color display) only accept numbers. After entering the desired number, the <ENTER> key move the cursor to the next input field. Parameter data fields (which are yellow on a color display) accept both numbers and parameter names, and are discussed in greater detail below.

3.2.3 Specifying Parameters

Recalling the discussion in Section 2.2, one of the greatest strengths of the RIP methodology is the fact that the software allows most input to be defined by the user as constants, stochastics, functions, or tables. This is carried out by specifying an alphanumeric parameter name (as opposed to a number) in a parameter data field.

Parameters are defined and edited through the "parameters module" of RIP, which is discussed in detail in Chapter 4. The parameters module contains a database of parameters defined by the user. The user may define as many parameters as deemed necessary. Defining a parameter consists of specifying a name, a type (e.g., constant, stochastic, function), and a form (e.g., a value, a specified distribution, or a specified function or dependency).

The parameters module is entered automatically by typing a parameter name in a parameter data field within any input window and hitting <ENTER>. If the parameter name specified in the parameter data field exists in the parameters module database, the parameters module editing window is displayed. As an example, consider the "mass transfer" window shown above. In this case, FLOW happens to be the name of a previously defined parameter. Moving the cursor to this parameter data field and hitting <ENTER> provides access to the parameters module and allows that parameter to be edited:

Repository Integration Program (Rev. 4.04)		
General	PA Model	Strategy Model
User's Guide Tutorial		
Waste Package Database Editor		
ID : HLDW	Package 2 of 2	F1=Prev F2=Next
DESC: vitrified waste		
Parameter Editing		
Identifier : FLOW Description: repository flow rate Parameter Type : Stochastic (log- Uniform : frcm 1 to 100) Save Time History : No Edit Parameter Definition [Affects]- [Function of]-		
F7=Display Dist. F8=Expected Value		

Note that <ESC> exits the parameters editing window and returns the user to the original input window. For all parameter data fields, RIP displays the expected value of the parameter to the right of the field in parentheses (if the parameter is constant, "Constant" is displayed).

The details of parameter editing are provided in Chapter 4. As will be discussed in detail in that chapter, in addition to entering the parameters module as described above, the parameters module can be entered directly from anywhere within the user interface using the hot-key <Alt>-<P>.

3.2.4 The On-Screen HELP Utility

RIP provides an on-screen HELP utility which provides explanations, warnings, and reminders to the user regarding various input windows or fields. The HELP utility is entered automatically by hitting <Alt>-<H>. Note that the user is reminded of this at the bottom of every screen (although this is not shown on the screens reproduced for this report).

RIP has three levels of HELP. The lowest level pertains to the particular input field at which the cursor is located when the user presses <Alt>-<H>. If a help screen exists for that field, it is displayed. For example, hitting <Alt>-<H> from within the [Waste Package] input window (described in Section 5.1.2) while the cursor is on *Number of Packages*, calls up the following help screen:

Repository Integration Program (Rev. 4.04)		
General	PA Model	Strategy Model
User's Guide Tutorial		
ID : H DESC: v Number MTHM pe Waste B Is mass Mass Tr Exposur Primary Seconda Invento Define (AE,1. Total D Total D	<h3>NUMBER OF WASTE PACKAGES</h3> <p>This is the number of waste packages of this particular type emplaced in the repository. This must be a non-negative integer.</p>	F1=Prev F2=Next F3=Add F4=Del F5=Copy F6=Copy Inventory
Alt-H:Window Help		

Note that, as indicated at the bottom of the screen, hitting <Alt>-<H> again calls up the second level of help, that which pertains to the entire window (in this case, the [Waste Package] window):

Repository Integration Program (Rev. 4.04)		
General	PA Model	Strategy Model
User's Guide Tutorial		
ID : H DESC: v Number MTHM pe Waste B Is mass Mass Tr Exposur Primary Seconda Invento Define (AE,1. Total D Total D	<h3>WASTE PACKAGE DESCRIPTION WINDOW</h3> <p>This window is used to describe the waste packages and their contents. All of the information must be specified for each waste package type to be included in the simulation.</p> <p>Specification of multiple waste package types allows the user to represent the different kinds of waste packages that will be emplaced in the repository (e.g., spent fuel, high level defense waste). This is necessary because different kinds of waste packages may behave quite differently (e.g., each type having different inventories, container failure rates, and/or mass exposure and mass transfer characteristics).</p> <p>The user can add waste package types with the <F3> key. Waste package types can be deleted with the <F4> key. The <F5> key copies all the data for the current waste package to a new waste package. The <F6> key copies the</p>	F1=Prev F2=Next F3=Add F4=Del F5=Copy F6=Copy Inventory
Alt-H:General Help PgDn		

Finally, as indicated at the bottom of the screen, hitting <Alt>-<H> a third time calls up the third and highest level of help, global instructions which pertains to the entire program:

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Repository Integration Program (Rev. 4.04)

Rnid	Decay Rate/yr	Half Life	Daughter	Sorption Group	Atomic Weight	Sp. Act. Ci/gram	Plot Color	Plot Line
AC227	3.18E-02	2.18E+01	-	1	227.00	7.23E+01	BLUE	DOTTED
AM241	1.60E-03	4.32E+02	NP237	1	241.00	3.44E+00	GREEN	CENTER
AM242	4.56E-03	1.52E+02	PU238	1	242.00	9.73E+00	CYAN	SOLID
AM242M	4.56E-03	1.52E+02	PU238	1	242.00	9.73E+00	RED	DOTTED
AM243	9.39E-05	7.38E+03	PU239	1	243.00	2.00E-01	MGENTA	CENTER
C14	1.21E-04	5.73E+03	-	1	14.00	4.46E+00	BROWN	SOLID
CA41	4.91E-06	1.41E+05	-	1	41.00	6.23E-02	LTGRAY	DOTTED
CL36	2.30E-06	3.01E+05	-	1	36.00	3.30E-02	DKGRAY	CENTER
CM243	2.43E-02	2.85E+01	PU239	1	243.00	5.17E+01	LTBLUE	SOLID
CM244	3.83E-02	1.81E+01	PU240	1	244.00	8.09E+01	LTGREN	DOTTED
CM245	8.15E-05	8.50E+03	AM241	1	245.00	1.72E-01	LTCYAN	CENTER
CM246	1.46E-04	4.73E+03	PU242	1	246.00	3.08E-01	LTRED	SOLID
CO60	1.32E-01	5.27E+00	-	1	60.00	1.13E+03	LTMGNT	DOTTED
CS135	3.01E-07	2.30E+06	-	1	135.00	1.15E-03	YELLOW	CENTER
CS137	2.31E-02	3.00E+01	-	1	137.00	8.71E+01	BLACK	SOLID

Press any key to switch to display of extra data
Use arrow-keys, PgUp/PgDn to scroll

As mentioned in Section 3.1.1, additional data can be stored in the species table for use in other portions of the front-end. By striking any key, these additional columns can be viewed here, as shown below.

Repository Integration Program (Rev. 4.04)

Rnid	MIMIC	ACTIVITY
AC227	0.00E+00	0.00E+00
AM241	0.00E+00	0.00E+00
AM242	2.00E+00	0.00E+00
AM242M	2.00E+00	0.00E+00
AM243	2.00E+00	0.00E+00
C14	0.00E+00	0.00E+00
CA41	0.00E+00	0.00E+00
CL36	0.00E+00	0.00E+00
CM243	0.00E+00	0.00E+00
CM244	9.00E+00	0.00E+00
CM245	9.00E+00	0.00E+00
CM246	9.00E+00	0.00E+00
CO60	0.00E+00	0.00E+00
CS135	0.00E+00	0.00E+00
CS137	1.40E+01	0.00E+00

Press any key to switch to display of basic properties
Use arrow-keys, PgUp/PgDn to scroll

H:Help F:Families G:General P:Parameters

3.2.6 Printing and Saving Input or Output Screens

For documentation purposes, the user may wish to print or save a screen capture of the input windows within the user interface. As will be discussed in subsequent sections, RIP provides several more powerful ways for documenting input (e.g., creating an echo file of the entire data set, discussed in Section 3.4; creating a listing of the parameter database, discussed in Section

4.2). Nevertheless, this utility may be useful for some users. Note that the windows reproduced in this document were created using this utility.

Printing and saving of screens is invoked automatically using the following key combinations:

- <Ctrl>-<P> sends the current screen to the printer. The user must specify the type of printer under the [General] window, discussed in Section 3.4.
- <Ctrl>-<F> sends the current screen to an ASCII file named SCREENS.DAT. The user is given the choice of adding the screen sequentially to the file, or overwriting the existing file.

Only *text screens* can be printed and saved in this manner. When running the front end on a PC with DOS 5.0 or above, it is possible to send graphics screens directly to the printer by typing <Shift>-<PrintScreen>. In order for this utility to be active, the GRAPHICS command should be added to the AUTOEXEC.BAT file. The type of printer must be specified as an argument for the GRAPHICS command (e.g., GRAPHICS LASERJETII). The user should refer to the DOS reference manual for more details.

3.2.7 Units

RIP is a dimensional model. That is, it requires that data be input using a specific set of data units. The actual units which are required for any given input field are specified in parentheses next to the field.

3.3 Entering Data and Applying RIP

For the most part, data are entered into RIP and a transfer file can be created by sequentially stepping through the menus and input windows of the user interface. The user begins by entering data in the input windows under [PA Model]. When editing an existing data input set, the user can move through the various input windows in any manner desired. Because of the interdependency of several of the input windows describing the PA model, however, when first defining a problem, the user must move through the windows in a specified order (as will be described in detail in Section 5). If just running the performance assessment model, the user can then create a transfer file from a window under [PA Model]. The back end program, which reads the transfer file and creates a results file, must then be executed. Post processing of results generated by the back end is carried out through the windows under [Results] in the user interface.

When evaluating alternative characterization strategies, in addition to the PA Model input, additional input must be entered in the [Strategy Model] input windows.

Note that while entering data in any part of RIP, the parameters module can be entered in several ways (as will be described in detail below) to define any parameters specified in the input windows.

We have briefly discussed above three of the four top level menu items in the user interface: [PA Model], [Strategy Model], and [Results]. The fourth top level menu item, [General], provides access to a window used for specifying some global input parameters. Several of these fields pertain to user utilities (e.g., allowing the user to specify the type of printer to which the user interface is attached; allowing the user to create an ASCII echo file of the entire input data set). The remaining input fields pertain to the details of the computational algorithm and sampling scheme.

The RIP user interface and the various input windows are discussed in detail below. The [General] input window is described in Section 3.4. The parameters module is then discussed in Chapter 4. Chapters 5 and 6 describe the performance assessment model and the strategy evaluation model, respectively. Finally Chapter 7 describes the post-processing of results.

3.4 Editing the [GENERAL] Input Window

The input window accessed by selecting [GENERAL] from the top level menu consists of the following input fields:

```

[■]-----Repository Integration Program (Rev. 4.04 )-----
      General      PA Model      Strategy Model      Results
      User's Guide Tutorial
[■]-----General Data-----file date: 08-14-95 15:35:21-----
Printer Type           : Laserjet II
Graphics Displays      : Color
Use Latin-Hypercube sampling? : No
Show M-C confidence bounds? : No
Repeat sampling sequences? : No
Species-table file     : rntable.dat
Values to use for Parameter Evaluation :
  Time : 0             WP Group : 1
Create Echo File
Available Memory       : 307652
F1 = Clear Parameter Importance Sampling
```

Printer Type - This is an option field (it blinks). It is required in order to print the current screen (using <CTRL>-<P>). The current version of RIP provides the user with three choices: Epson LX, HP Laserjet, and HP Laserjet II. Press <PgUp> or <PgDn> to select the appropriate printer. Note that more recent HP Laserjet models (e.g., Laserjet III, Laserjet IV) are supported using the Laserjet II option.

Graphics Displays - This is an option field with two choices: color, or monochrome. Press <PgUp> or <PgDn> to select the appropriate choice. For several types of graphics displays produced by RIP, color plots are much easier to view. When just using screen graphics, always choose color. When making a hardcopy plot to a black and white printer, however, it is better to choose monochrome. This is because for several types of display, the program uses different line types (to substitute for colors) so that they can be distinguished in a monochrome hardcopy plot.

Use Latin-Hypercube sampling - This option field specifies whether or not Latin-Hypercube sampling will be used within the Monte Carlo sampling scheme. It is answered Yes or No. Latin-Hypercube sampling is discussed in detail in Appendix C of

the RIP Theory and Capabilities Manual. Note that the use of Latin-Hypercube sampling can be used whether or not importance sampling is being implemented.

Show M-C confidence bounds? - This option field specifies whether or not to show confidence bounds when displaying Monte Carlo results. This applies to both parameters (viewed from within the Parameters Module) and to RIP results (viewed from the post-processor). The theory behind the computation of confidence bounds is discussed in Appendix C of the RIP Theory and Capabilities Manual. Note that confidence bounds cannot be used if importance sampling is used.

Repeat sampling sequences - This option field specifies whether a repeatable random number sequence is to be used. Answering No creates a new random number sequence for sampling. Answering Yes results in the use of a repeatable random number sequence (allowing simulations to be repeated exactly).

Species-table file - This field contains the name of the user-defined ASCII file specifying the species to be included in the simulation (see Section 3.1.1). If the user changes the species table file, it is necessary to exit and reenter RIP (so the new file can be read in and the data set is reconfigured).

Values to use for Parameter Evaluation - As discussed in detail in Section 4.3.2, the parameters module allows parameters to be described as a function of several internally-defined, reserved parameter names (TIME, TEMP, CONTAC, and user defined environmental factors). The two fields directly below this line (*Time* and *WP Group*) are used to specify how the parameters module will evaluate parameters which are explicit functions of these reserved names. (As discussed in Section 5.1.1, the waste package group defines the values for TEMP, CONTAC, and other environmental factors). The values specified here are only used during parameter evaluation within the parameters module (i.e., when using the <F7> and <F8> keys).

Create Echo File - This access field allows the user to create an echo of the current input file. This is an ASCII file which summarizes all input, providing documentation for the run. A pop-up window prompts the user for the name of the file to be created. Specifying a name and hitting <ENTER> immediately creates the new echo file.

Available Memory - This field displays the amount of memory currently available. This field differs slightly from the available memory field at the top of the RIP main window. The field on the main window reflects the amount of available memory at the time that the current RIP session is entered. The field in the [General] menu shows the exact amount available at the current time. By comparing the two values, the user can determine how much memory is being used by the open RIP menus, or, if running under Windows, by other Windows applications that have been opened.

The <F1> key can be used to globally reset stochastic sampling bias. As discussed in detail in Appendix C of the RIP Theory and Capabilities Manual, RIP utilizes an *importance sampling scheme* to increase the efficiency of the Monte Carlo sampling process. The user can choose the degree to which importance sampling is to be used (i.e., the amount of sampling bias) on any

given parameter. As will be discussed in detail in Chapter 4, the level of biasing for each parameter can be specified separately within the parameters module. The <F1> key allows the user to globally reset the level of biasing for all parameters to None (i.e., no bias). No Bias results in straight Monte Carlo sampling without importance sampling.

Note that the user can enter the [GENERAL] input window directly from the top level menu or indirectly from anywhere within the user interface by pressing <Alt>-<G>.

4. DEFINING PARAMETERS

As described in Sections 2.2 and 3.2.3, the *parameters module* is the cornerstone of the RIP methodology, and consists of a library of computer procedures designed to assist in numerical simulations of complex, stochastic systems. The fundamental concept is that the symbols used to express the parameters of an equation can refer to a variety of alternative types of parameters. A parameter can be represented as:

1. a constant;
2. a stochastic (uncertain) variable;
3. a table of values;
4. a function of other parameters; or
5. an event.

The RIP user could, for example, define a parameter Y using the following equation:

$$A * X + B$$

where:

- A is a stochastic parameter, with a log-normal probability distribution;
- X is a function of some additional parameters (e.g., $X = D * Z$); and
- B is a constant.

The parameter Y would also be stochastic, since it is a function of one or more stochastic parameters. Using the parameters module, the above equations, the probability distributions of the stochastic parameters, and the values of the constants can be directly entered by the user. The user can then compute and display the probability distribution of Y, along with its subsidiary parameters A and X.

The parameters module allows the user to develop a database of parameter definitions. In addition, having defined a parameter, and prior to actually running the repository system simulation using RIP, the user can evaluate and display the value (for a deterministic parameter) or the probability distribution (for a stochastic parameter). Entry and editing of data is straightforward. The user enters the symbolic name for each parameter, and types in the equation (for a function), the type and form of the probability distribution (for a stochastic parameter), a set of data points against an independent parameter (for a table), or the value (for a constant). In addition, the software is configured so that complex coded-functions (user-defined modules written in the C programming language, whose output parameters become RIP parameters) can be directly linked into the parameter database.

The nature of the parameter types, the facilities to enter and edit parameter data, and the means of generating graphical representations of stochastic parameters are presented in the following sections.

4.1 Entering the Parameters Module

The parameters module can be entered in two ways:

- It is entered automatically by typing a parameter name in a parameter data field in any input window and hitting <ENTER>. If the parameter name specified exists in the parameter module database, the parameters module editing window is displayed. If the parameter name does not exist, RIP will ask whether the user wishes to add it to the database. If the answer is *Yes*, the parameters editing window is then displayed. If the answer is *No*, the parameter is not added to the parameters database (the user will need, however, to add the parameter to the database prior to running a simulation).
- The parameters module can also be entered directly from anywhere within the user interface by hitting <Alt>-<P>.

4.2 Browsing and Editing the Parameter Database

The parameter module editing window is illustrated below:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Parameter Editing			
Identifier : A1		Parameter No. : 1 of 35	
Description: log-uniform distribution			
Parameter Type : Stochastic			
(Uniform : from 1 to 10)			
Save Time History : No			
Edit Parameter Definition			
[Affects] -A2,A3,EA1			
[Function of]-			
F1=Prev Param	F2=Next Param	F3=Add Param	F4=Delete Param
F5=Find Param	F6=Print Summary	F7=Display Dist.	F8=Expected Value
F9=Strategy	F10=Bayesian update (Current update level=0)		

The parameter database is ordered alphabetically by name. If the parameter editing window is entered using <Alt>-<P>, it will display the first parameter in sequence. If the editing window is entered indirectly by typing a parameter name within a parameter field and hitting <Enter>, it will display the specified parameter. The user can browse through the database and perform editing operations using the function keys:

- F1 Move to previous parameter in alphabetic order
- F2 Move to next parameter in alphabetic order
- F3 Insert a new parameter
- F4 Delete the current parameter
- F5 Find a specific parameter by name
- F6 Print a summary of the database
- F7 Display the distribution of a stochastic parameter or function

- F8 Display the expected value of a stochastic parameter
- F9 Determine the effect of a specified characterization strategy on the parameter
- F10 Carry out a Bayesian update

Note that if the parameters module is entered indirectly (by specifying a parameter name and hitting <ENTER>), only the <F7> and <F8> are active. This is because when the parameters module is entered in this manner, only the parameter that has been specified can be edited. The parameters module must be entered directly using <Alt>-<P> to have full access to the entire parameters database. (Note, however, that when entering the parameters unit from within the post-processor, the <F3>, <F4>, <F7>, <F9>, and <F10> keys are inactive.)

Functions keys <F1> and <F2> allow you to move backwards and forwards through the database in alphabetical order.

The <F3> key allows a new parameter record to be created. The user is prompted for the name of the new parameter to be created. The user can enter values for the new parameter as described below in Section 4.3. The default form for a newly created parameter is a constant with a value of 0.

If the name of the new parameter is followed by "=", the new parameter is created as a direct copy of the parameter which was on the screen when <F3> was pressed. This is useful for creating new parameters which are only slightly different from existing parameters.

The <F4> key is used to delete parameters from the database. When you press the <F4> key, a window will pop up with the query:

"Confirm deletion of parameter NAME: (Y):"

Press "Y" or <Enter> to confirm the deletion. Press "N" if you want to change your mind.

The <F5> key is used to find a parameter within the database. When you press the <F5> key, a window will pop up to prompt you for the ID of the parameter you wish to find and edit. Type all or part of the ID, press <Enter>, and the data for the selected parameter will be displayed ready for editing. If you enter a number, rather than a parameter name, the data for the selected parameter number will be displayed. In either case, an error message will appear if no matching parameter can be found in the database.

The <F6> key is used to print a summary of the parameters database. When you press the <F6> key, a window will pop up with the query

"Do you want detailed parameter output? (N):"

Press "Y" or <Enter> for a detailed listing of all parameters. Press "N" for a short listing (one line for each parameter). The detailed listing goes to a file named PARAM.DET. The short listing goes to a file named PARAM.GEN. You can send these files to your printer after leaving the parameters program.

The <F7> key is used to display the distribution of a stochastic parameter or function. This is described in more detail in Section 4.4 below.

The <F8> key displays the expected value of parameters. For function parameters, RIP displays the value of the function based on the expected values of the parameters on which it is dependent. *Note that this is not necessarily equal to the expected value of the function.* To compute the true expected value of a function, you must use the <F7> key. If the parameter is a function of TIME or near-field environmental factors, the values for TIME and WP Group specified in the GENERAL window are used when evaluating the function for the expected value.

The <F9> key computes the effect of a strategy on a parameter, and is discussed in detail in Chapter 6.

The <F10> key is only active for stochastic parameters, and is discussed in more detail in Section 4.3.3.2.

Note that while in the parameters module, the user can use <Alt>-<L> to provide a quick listing of the parameters within the database. The user can list the names of all parameters, the names along with a short description, and, if desired, list stochastic, function, and event parameters separately.

4.3 Editing Parameters

The arrow keys (or the <TAB> and <SHIFT>-<TAB> keys) can be used to move between fields which can be edited in the parameter window. Within a field, the left and right arrow keys, and the <Home> and the <End> keys can be used for movement. The <Ins>, <Delete> and <Backspace> keys can also be used for editing fields. The various input fields are described below:

Identifier - The first two input fields are descriptive fields. The first highlighted field is the *Identifier*. This is the six character name or ID for the parameter. Note that there are a number of character strings that the user interface will not allow. This is discussed in more detail in Section 4.3.2. Once a parameter has been defined, this field can not be edited (although the parameter can be deleted if desired).

Description - This is a short description of the parameter.

Parameter Type - Within this option field, the user can select one of the following parameter types: 1) constant; 2) function; 3) stochastic; 4) table; or 5) event.

Save Time History - This option field allows the user to indicate whether or not time history information is saved for the current parameter. It is often valuable to observe the values of individual parameters that change as a function of time. If "yes" is selected, the

value of the parameter will be saved at each time step and will be available for viewing in the post-processor.

Edit Parameter Definition- This field provides access to a variety of pop-up windows and is used to enter or modify the definition of a parameter. There are several such windows; one for each type of parameter. These windows are discussed individually in the following sections.

Note that directly above *Edit Parameter Definition*, the actual definition of the parameter is displayed. This allows the user to quickly view the parameter definition. Directly below *Edit Parameter Definition*, RIP displays what other parameters the current parameter *Affects* or is a *Function of*. Parameters which the current parameter "affects" are dependent on (i.e., a function of) the current parameter. The current parameter is dependent on those parameters which are listed under "function of".

Note that the "affects" and "function of" parameter lists can be viewed in two ways. First, they are listed directly below the *Edit Parameter Definition* field. Since only a limited number of parameter names can fit on the screen, however, the entire list can also be viewed by moving to the *Affects* or *Function of* access fields and pressing <ENTER>:

Two important points regarding definition of parameters must be noted. First, if a parameter definition refers to another parameter name, that parameter must be edited separately. For example, if parameter A is defined as $B + C$, and parameters B and C are undefined, the user must define these parameters separately after completing the definition for A. New parameters can be defined by invoking the parameters module using <Alt>-<P> and using the <F3> key. RIP will warn the user if the parameter definition has referred to undefined parameters. *RIP will not create a transfer file if undefined parameters are referenced in the parameters database.*

The second point is related to the first, but somewhat more subtle. Namely, *recursive definition of parameters is not allowed*. Referring to the example mentioned above, if A is defined as a function of B and C, B and C can not be defined as a function of A. Such a definition would be recursive and,

although in some cases it might be mathematically consistent (e.g., requiring the solution of simultaneous equations), it is not allowed in RIP.

4.3.1 Defining a Constant Parameter

When the user selects [Edit Parameter Definition] for a constant parameter, a window labeled "Edit Constant" will appear:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Parameter Editing			
Identifier : AREA		Parameter No. : 5 of 38	
Description: repository area			
Parameter Type : Constant (5600000)			
Save Time History : No		[Edit Constant]	
Edit Parameter Definit		5600000	
[Affects]-			
[Function of]-			
F1=Prev Param F2=Next Param F3=Add Param F4=Delete Param			
F5=Find Param F6=Print Summary F7=Display Dist. F8=Expected Value			
F9=Strategy F10=Bayesian update (Current update level=0)			

The user can use the right and left arrow keys, the <Home> and the <End> key for movement within this field. The <Insert>, <Delete> and <Backspace> keys can be used for editing. When the correct value has been entered, use the <Enter> key to close the "Edit Constant" window and return to the main parameter editing screen. If the parameter value has been modified, hitting the <Esc> key will undo the change and restore the original value. Hitting <Esc> a second time will close the window.

4.3.2 Defining a Function Parameter

Function type parameters impart a tremendous amount of flexibility to the parameters module. Function type parameters can be described directly as functions of other parameters. In the two examples shown here, the parameters are defined as functions of three other user-defined parameters (A, B, and C):

example 1: IF(A >= 10, B,C)

example 2: (A + B) * LOG(C)

When the user selects [Edit Parameter Definition] for a function parameter, a window labeled "Edit Equation" will appear:

Repository Integration Program (Rev. 4.04)

General
PA Model
Strategy Model
Results

Parameter Editing

Identifier : B

Description: function of time

Parameter Type : Function

[if(time==100,10,100)]

Parameter No. : 6 of 38

Sa [] Edit Equation

Ed [if(time==100,10,100)]

[A]

{Function of}-TIME

F1=Prev Param F2=Next Param F3=Add Param F4=Delete Param

F5=Find Param F6=Print Summary F7=Display Dist. F8=Expected Value

F9=Strategy F10=Bayesian update (Current update level=0)

The equation that defines a function parameter can be up to 40 characters in length. No distinction is made between upper and lower case in equations. Equations can include blank spaces, which are ignored. Equations can include parameter ID's, numeric constants and built-in functions. The following mathematical operators are allowed:

Table 4-1. Summary of Supported Function Operators

Operator	Function
<i>Mathematical Operators</i>	
+	addition
-	subtraction
/	division
*	multiplication
**	exponentiation
()	parenthesis for grouping
<i>Relational Operators</i>	
==	equal to
<>	not equal to
>	greater than
<	less than
>=	greater than or equal to
<=	less than or equal to
!!	or
&&	and
!	not

Expressions using relational operators are evaluated as to whether they are true or false. If the expression is true, it takes on the value of 1; if it is false, it takes on the value of 0. An expression which consists of a value is considered true for all values other than zero. Hence, 1&&1 is equal to 1 (it is a true statement); 1&&0 is equal to 0 (it is false since 0 is equivalent to a false

statement). Note that !0 is equal to 1 (a true statement); !(any non-zero value) is equal to 0 (a false statement).

Table 4-2 is the list of operators, shown in order the in which they are evaluated in a function statement. For example, in the function statement:

$$A + B * C$$

B times C would be evaluated first, then A would be added to that quantity because the "*" operator has a higher precedence level than "+" operator. However, (A+B)*C would result in a different value because the "()" symbols have higher precedence than the "*" operator.

Table 4-2. Precedence Levels for Each Operator

Precedence Level	Classification	Operators
1	parentheses	()
2	unary	!
3	multiplicative	*, /
4	additive	+, -
5	relational	>, <, >=, <=
6	equality	==, <>
7	logical AND	&&
8	logical OR	!!

RIP also supports several built-in functions, which are summarized in Table 4-3.

Table 4-3 List of Supported Functions

Function	Description
<i>Trigonometric Functions</i>	
SIN(A)	Returns the sine of A, with A given in radians
COS(A)	Returns the cosine of A, with A given in radians
TAN(A)	Returns the tangent of A, with A given in radians
COT(A)	Returns the cotangent of A, with A given in radians
ASIN(X)	Returns the arcsine, in radians, of A
ACOS(X)	Returns the arccosine, in radians, of A
ATAN(X)	Returns the arctangent, in radians, of A
SINH(X)	Returns the hyperbolic sine of A, with A given in radians
COSH(X)	Returns the hyperbolic cosine of A, with A given in radians
TANH(x)	Returns the hyperbolic tangent of A, with A given in radians
<i>General Functions</i>	
ABS(X)	Absolute value of X
BESS(V,X)	Bessel function of X of order V
BETA(X,Y)	Beta function
ERRF(X)	Gauss error function of X
EXP(X)	Exponential (e^x)
IF(X,Y,Z)	If X is True, Then Y, Else Z
LN(X)	Natural logarithm of X
LOG(X)	Logarithm base 10 of X
MAX(X,Y)	Returns the max of X and Y
MIN(X,Y)	Returns the min of X and Y
RAND	Returns a random number between 0 and 1
SQRT(X)	Square root of X
TABLE(X1, X2,...,Xn,#)	Multi-dimensional lookup table (discussed in section 4.3.5)

As shown in the Table 4-3, IF-THEN logic is supported, in which X, Y, and Z are parameters, expressions, or functions. The IF function is interpreted as follows: if X is not equal to 0 (i.e., if X is a true expression), then the function is equal to Y, otherwise it is equal to Z. Specifying the first argument as an expression using relational operators, and nesting the function permits a large degree of flexibility. For example,

IF(X==1,Y,(IF(X==2,Z,ZZ))) says the following:

```
if X = 1
    the function = Y;
else
    if X = 2
        the function = Z;
    else
        the function = ZZ
    endif
endif
```

There is no limit to the degree of function nesting.

The last built-in function listed in Table 4-3, the multi-dimensional lookup table, will be discussed separately, in section 4.3.5.

When you have completed editing the function definition, press the <Enter> key to close this window and return to the main parameter editing window.

In addition to defining parameters such that they are dependent on other user-defined parameters, the user can also define parameters which are described in terms of several *internally-defined, reserved parameter names*. In particular, the user can refer to the following parameter names, summarized in Table 4-4:

Table 4-4 Reserved Parameter Names

Parameter Name	Description
TIME	the simulation time
TEMP	the time-varying temperature at the edge of a waste package
CONTAC	the water contact mode at a particular waste package
" ____ "	the names of any user-defined environmental factors defined under [Near Field Conditions]

Use of TIME is straightforward. If the user wishes to describe a process with a parameter which changes with time (TIME=0 being the start of the simulation), that parameter can be described as a function of time (in years).

The other names listed above refer to *environmental factors*, which describe *near field conditions* in the immediate vicinity of a waste package (e.g., temperature, moisture, or chemical conditions). These environmental factors can only be referenced in parameter definitions which pertain to waste package behavior (in particular, those input fields accessed under the [Waste Package Description] menu option). They are described in detail in Section 5.1.1.

Unlike the environmental factors, TIME can be referenced throughout the user interface. Not all input variables, however, are allowed to be specified as functions of time. In some cases, this is due to computational considerations associated with the algorithms implemented within RIP; in others it is not physically reasonable to describe the input in such a manner. Inputs that are constrained in this manner are clearly noted in the following chapter. As will be shown in Section 5.1.1, TEMP is defined by the user as a function of time. Therefore, any inputs that are constrained to being temporally invariant can not be described as a function of TIME or TEMP. The user interface automatically checks for these constraints prior to creation of the transfer file.

Note that although TIME, TEMP and other environmental factors can be referenced within a parameter definition as discussed above, *they can never be entered directly into a parameter input field in the RIP interface* (since the user interface expects either a number or a parameter name).

RIP will not allow the user to define parameters having the names listed above. These names are *reserved*. Likewise, operator names included in the user-interface equation parser (e.g., IF, COS, LOG) are also reserved.

Note that it is possible to obtain lists of all parameters which are dependent on the reserved parameters (TIME, TEMP, CONTAC, other factors) by pressing <Alt>-<A> from within the parameters unit. The following window will be displayed:

Repository Integration Program (Rev. 4.04)

General PA Model Strategy Model Results

Parameter Editing

Affects lists for Time and Environmental Factors

Parameters affected by TIME :

B

Parameters affected by TEMP :

Parameters affected by CONTAC :

FF

Parameters affected by other environmental factors : 1 of 1

Factor ID : PH

FG

F1-NEXT FACTOR F2=PREVIOUS FACTOR

4.3.3 Defining a Stochastic Parameter

When the user selects [Edit Parameter Definition] for a stochastic parameter, a "Probability Distribution Definition" window will appear. An example of this window appears below:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Parameter Editing			
Identifier : A1		Parameter No. : 1 cf 37	
Description: log-uniform distribution			
Parameter Type : Stochastic			
(Uniform : from 1 to 10)			
<div style="border: 1px solid black; padding: 5px;"> <div style="display: flex; justify-content: space-between;"> [■] UNIFORM DISTRIBUTION </div> <div style="display: flex; justify-content: space-between;"> <div> Save Time Edit Param [Affects [Function </div> <div> Sampling Bias : No Bias linear Lower bound: 1 Upper bound: 10 </div> <div> F1=Prev type F2=Next type F3=Log/Linear (Constant) (Constant) </div> </div> </div>			
F1=Prev Param F2=Next Param F3=Add Param F4=Delete Param F5=Find Param F6=Print Summary F7=Display Dist. F8=Expected Value F9=Strategy F10=Bayesian update (Current update level=0)			

Pressing the <F1> or <F2> key will switch between the distribution types summarized in Table 4-5. Appendix A discusses the form and required inputs for each of these distributions in detail.

As is described in Appendix A, the fields that appear in the "Probability Distribution Definition" window will change with the distribution type. For example, the window for a normal distribution includes fields for the mean and standard deviation of the distribution, while a triangular distribution is defined by fields for lower bound, upper bound and most likely value. In any of these fields, the user can enter either a numeric constant or the name of another parameter. If one of the fields that defines a probability distribution contains the name of another parameter, that parameter must be edited separately.

RIP does not allow stochastic parameters to be described as a function of time. Hence, for a stochastic parameter which has been specified using a normal distribution, the mean and the standard deviation cannot be described as a function of time. This limitation has been imposed to minimize improper use of stochastic parameters.

Table 4-5 List of Supported Probability Distributions

Beta
Binomial
Boolean
Cumulative
Determinate
Discrete
Gamma
Truncated Gamma
Normal
Truncated Normal
Lognormal
Truncated Lognormal
Poisson
Triangular
Log-Triangular
Uniform
Log-Uniform
Weibull
Truncated Weibull

4.3.3.1 Sampling Bias

Every stochastic parameter input window has a "*Sampling Bias*" input field. This refers to the amount of importance sampling (or biasing) which is to be used when sampling the distribution. The user has four choices to toggle through: No Bias, Low Bias, Medium Bias, and High Bias. No Bias is the default. No Bias results in straight Monte Carlo sampling with no importance sampling. The other three choices represent increasing levels of importance sampling. The sampling bias for all parameters can be reset to No Bias by hitting <F1> in the [General] menu. Biasing is discussed in detail in Appendix C of the RIP Theory and Capabilities Manual. Using the importance sampling terminology defined in that appendix, the biasing is specified in RIP as shown in Table 4-6.

Table 4-6 Summary of Sampling Bias Definitions

Bias Level	Bias Exponent
No Bias	n=1.00
Low Bias	n=1.33
Medium Bias	n=1.67
High Bias	n=2.00

4.3.3.2 Bayesian Updating Stochastic Parameters

The <F10> key in the main parameter window allows the user to create (and view) a Bayesian update of a stochastic parameter (this key is only active for stochastic parameters). This feature is added to illustrate the Bayesian updating scheme incorporated into the strategy model. Bayesian updating is discussed in detail in Chapter 7 of the RIP Theory and Capabilities Manual and Chapter 6 of this document.

The following pop-up window is displayed upon hitting the <F10> key:

Repository Integration Program (Rev. 4.04)																											
General	PA Model	Strategy Model	Results																								
Parameter Editing																											
Identifier : A1	Parameter No. : 1 of 37																										
Description: log-uniform distribution																											
Parameter Type : Stochastic																											
(Uniform :	<table border="1"> <thead> <tr> <th colspan="3">BAYESIAN UPDATE</th> </tr> <tr> <th>Lower bound</th> <th>Test result</th> <th>Upper bound</th> </tr> </thead> <tbody> <tr> <td>1.000009</td> <td>5.5</td> <td>9.99999</td> </tr> <tr> <td colspan="3">Current standard deviation (σ): 2.598076</td> </tr> <tr> <td colspan="3">Ratio of test σ to current σ : 1</td> </tr> <tr> <td colspan="3">(smaller values represent more information)</td> </tr> <tr> <td colspan="3">Press 'Enter' to Execute Update</td> </tr> <tr> <td colspan="3">(current update level= 0)</td> </tr> </tbody> </table>			BAYESIAN UPDATE			Lower bound	Test result	Upper bound	1.000009	5.5	9.99999	Current standard deviation (σ): 2.598076			Ratio of test σ to current σ : 1			(smaller values represent more information)			Press 'Enter' to Execute Update			(current update level= 0)		
BAYESIAN UPDATE																											
Lower bound	Test result	Upper bound																									
1.000009	5.5	9.99999																									
Current standard deviation (σ): 2.598076																											
Ratio of test σ to current σ : 1																											
(smaller values represent more information)																											
Press 'Enter' to Execute Update																											
(current update level= 0)																											
Save Time Hist																											
Edit Parameter																											
[Affects]-																											
[Function of]-																											
F1=Prev Param	F1=Pop Update	e Param																									
F5=Find Param	F6=Print Summary	F7=Display Dist.	F8=Expected Value																								
F9=Strategy	F10=Bayesian update (Current update level=0)																										

The "Lower bound", "Upper bound", and "Current standard deviation" fields can not be edited by the user. They display the lower and upper bounds, and the standard deviation of the current distribution. The user must select a "Test result" that is somewhere between the two bounds. This test result represents the value of the parameter implied by new information (when actually evaluating the effect of a strategy, RIP randomly samples this value.) The "Ratio of test σ to current σ " specifies the precision of the "new information" relative to that represented by the original distribution (the "old information" or prior knowledge). Specifying 0.1 implies that the new information is ten times more precise than the old information (i.e., the standard deviation of the new information is a tenth that of the old); specifying 2 implies that the new information is only half as precise as the old information. A new updated distribution is then created by moving the cursor to "Press 'Enter' to Execute Update" and hitting <Enter>.

The updated distribution can be viewed (using the <F7> key). Note that the updated distribution is *always in the form of a cumulative distribution*, regardless of the form of the original distribution.

After updating a parameter the display field named "current update level" on the parameter editing screen will change (from 0 to 1). Note that the current update level is also indicated within the Bayesian Update window illustrated above. If another update is carried out, this value becomes 2. The update level identifies the distribution that is "at the top of the stack" and which can currently be accessed and viewed. Additional updates update the previously

updated distribution. Hence update level 2 is an update of update level 1, which is an update of update level 0 (the original distribution). The user can "pop" down the stack (all the way back to update level 0) by hitting <F1> from within the Bayesian update window.

Note that the "Upper bound", "Lower bound", and the "Current standard deviation" displayed in the Bayesian Update window refer to the current update (which is not necessarily the original distribution).

Note that the <F10> option described here is intended only to illustrate the updating algorithm used in the strategy model. It does not affect the shape of the distribution used in performance simulations. The original distribution (update level 0) is always used for performance simulations (i.e., RIP automatically "pops" all the way back to level 0 prior to the simulation).

4.3.4 Table Parameters

An additional parameter type called a *Table* is available within the parameters unit (in addition to *Constant*, *Stochastic*, *Function*, and *Event*). A Table type parameter is a one-dimensional look-up table specified by the user. The window for entering a Table parameter is shown below:

Repository Integration Program (Rev. 4.04)

General PA Model Strategy Model Results

Parameter Editing

Identifier : TABLE Parameter No. : 4 of 5

Description: one-dimensional look-up table

Parameter Type : Table

(0)

Save Time His
Edit Paramete
[Affects]

TABLE DEFINITION

Interpolate
Linear
Linear

Dependent Parameter : TABLE
Independent Parameter: FUNC
Extrapolate beyond ends: Yes

	FUNC	TABLE
1 0	0	0
2 0	0	0
3 0	0	0
4 0	0	0
5 0	0	0
6 0	0	0
7 0	0	0
8 0	0	0
9 0	0	0
10 0	0	0

F1=Prev F2=Next F3=Plot

ete Param
ected Value
)

Table parameters are defined by first specifying the independent parameter upon which the dependent parameter (i.e., the parameter being defined) depends. The independent parameter can be any previously defined RIP parameter.

The user can define up to 25 data pairs. Only 10 data pairs are shown on the screen at once. The <F1> and <F2> keys can be used to move upward or downward through all 25 pairs.

RIP will interpolate between the entered data points in order to determine the value of the dependent parameter for a given value of the independent parameter. For each axis (i.e., the

independent and the dependent parameter), the user must specify whether the interpolation will be carried out linearly or logarithmically.

For calculating the dependent parameter in cases where the value of the independent parameter is beyond the range of the entered data, the user must specify whether or not RIP should extrapolate beyond the ends of the input data. If the user chooses not to extrapolate, the dependent parameter is fixed at the first (or last) value specified by the user for all values of the independent parameter which are beyond the range of the input data. If the user chooses to extrapolate, RIP uses the first two (or last two) data points to extrapolate backward (or forward). Note that the user should exercise caution if choosing to extrapolate, as this could result in unrealistically small (or large) numbers.

The <F3> key creates a screen plot of the dependent parameter as a function of the independent parameter.

4.3.5 Multi-Dimensional Look-up Tables

In addition to the one-dimensional lookup tables, RIP also allows the user to define multi-dimensional lookup tables.

Whereas a one-dimensional look-up table defines a line, a multi-dimensional look-up table defines a multi-dimensional surface. Hence, an n -dimensional look-up table defines the surface $f(x_1, x_2, \dots, x_n)$, where x_1 through x_n are the independent variables. $f(x_{1,1}, x_{2,1}, \dots, x_{n,1})$ represents the value of the dependent variable (i.e., the "result" of the table look-up) for specific values ($x_{1,1}, x_{2,1}, \dots, x_{n,1}$) of the n independent variables. RIP determines the value of $f(x_{1,1}, x_{2,1}, \dots, x_{n,1})$ by interpolating between look-up table data points supplied by the user.

The manner in which the look-up table is specified, referenced, and numerically implemented is described below.

4.3.5.1 Specifying the Look-up Table

As described above in Section 4.3.4, specification of a one-dimensional table is straightforward, as it is simply a set of points: $(x_1, f(x_1)), (x_2, f(x_2)), \dots, (x_n, f(x_n))$, where x_i is the value of the independent variable, and $f(x_i)$ is the value of the dependent variable. Specification of a multi-dimensional table is completely analogous, but involves more dimensions. The multi-dimensional table is specified by creating a separate ASCII file which can then be directly referenced by RIP. This is because the specification of a large multi-dimensional table using an input window similar to that for a one-dimensional table would be awkward.

The multi-dimensional look-up table is defined in an ASCII file that must be located in the same directory as the RIP code and input files. The file must be named TABLE*i*.TXT, where i can be 1, 2, 3, 4, or 5 (currently, up to 5 look-up tables can be defined).

The look-up table is specified in terms of a multi-dimensional grid of data points (analogous to a finite difference grid). The data points need *not* be uniformly spaced along a particular axis (i.e., the interval between points in any given dimension need not be uniform). Rather, the user specifies the values of each of the independent variables (i.e., each dimension) for which results will be defined. The manner in which this is done is most easily illustrated by considering an example.

Consider the two-dimensional table defined by the following points:

Table 4-7 Example Multi-Dimensional Lookup Table Points

Independent Parameter 1 [x_1]	Independent Parameter 2 [x_2]	Dependent Parameter [$f(x_1, x_2)$]
1	1	1
3	1	1.5
9	1	2.5
1	2	1.5
3	2	2
9	2	4
1	4	2.5
3	4	3
9	4	5
1	8	5
3	8	6
9	8	10

The first two columns define the "grid" (i.e., the locations of the data points). This particular example would define the following grid of data points:

Figure 4-1 Plot of Example Multi-Dimensional Lookup Table Points

Each grid point has associated with it a particular value for the dependent parameter (i.e., the third column in Table 4.1).

The format for specifying the look-up table in the ASCII file is as follows:

- number of dimensions:

n

- number of grid points in each dimension:

$p(1), p(2), \dots, p(n)$

- the values of the independent variable in each dimension:

$x_{1,1}, x_{1,2}, x_{1,3}, \dots, x_{1,p(1)}$

$x_{2,1}, x_{2,2}, x_{2,3}, \dots, x_{2,p(2)}$

.

.

.

$x_{n,1}, x_{n,2}, x_{n,3}, \dots, x_{n,p(n)}$

- the values for the dependent variable at the grid points:

$$\begin{aligned}
 &f(x_{1,1}, x_{2,1}, \dots, x_{n,1}), f(x_{1,2}, x_{2,1}, \dots, x_{n,1}), \dots, f(x_{1,p(1)}, x_{2,1}, x_{n,1}) \\
 &f(x_{1,1}, x_{2,2}, \dots, x_{n,1}), f(x_{1,2}, x_{2,2}, \dots, x_{n,1}), \dots, f(x_{1,p(1)}, x_{2,2}, x_{n,1}) \\
 &\quad \vdots \\
 &\quad \vdots \\
 &\quad \vdots \\
 &f(x_{1,1}, x_{2,p(2)}, \dots, x_{n,p(n)}), f(x_{1,2}, x_{2,p(2)}, \dots, x_{n,p(n)}), \dots, f(x_{1,p(1)}, x_{2,p(2)}, x_{n,p(n)})
 \end{aligned}$$

The order in which the values for the dependent variable are entered is most clearly seen by considering the following nested loop, which schematically illustrates how the data is actually read into the program:

```

DO i(n)= 1, p(n)
  DO i(n-1) = 1, p(n-1)
    .
    .
    .
    DO i(1)= 1, p(1)
      read f(xi(1), xi(2), ..., xi(n))
    ENDDO
    go to next line
    .
    .
    .
  ENDDO
ENDDO

```

As can be seen, the first independent variable varies the quickest (i.e., it is the innermost loop), while the last independent variable varies the slowest (i.e., it is the outermost loop). Note that the total number of independent values that are read must be equal to the product of $p(1)$ through $p(n)$.

The manner in which the ASCII file would be specified for the example look-up table defined in Table 1 is shown below:

! Example ASCII file

```

2
3 4
1 3 9
1 2 4 8
1 1.5 2.5
1.5 2 4
2.5 3 5
5 6 10

```

Note that comment lines may be inserted anywhere within the data file, but must begin with an "!".

4.3.5.2 Referencing the Look-up Table

The look-up table can be referenced when defining a function parameter by using the special TABLE operator. The TABLE operator has $n+1$ arguments, where n is the number of independent parameters in the look-up table. The first n arguments list the values for the independent parameters for which a result is to be interpolated. The last argument refers to the ASCII file which contains the data for the look-up table.

For example,

TABLE(A,B,1)

is interpreted as follows:

1. Use the two dimensional look-up table specified in the ASCII file TABLE1.TXT
2. Interpolate a value from the table using A as the value for the first independent variable, and B as the value for the second independent variable.

Note that A and B in this example are existing parameters in the database.

4.3.5.3 Interpolating from the Look-up Table

This section briefly describes the manner in which RIP interpolates within the table. Given a point in the n -dimensional space for which the value of the dependent variable must be evaluated, the following steps are carried out:

1. Determine the hypercube within the grid of table data points in which the point to be evaluated falls. Note that for a two-dimensional table, the hypercube is simply a rectangle. For a three dimensional table, it is a cube.
2. "Collapse" from n dimensions to $n-1$ dimensions by linearly interpolating between points in the first independent parameter dimension. This must be done 2^{n-1} times (i.e., along each edge of the hypercube that is parallel to the dimension being collapsed). This reduces the number of data values in the hypercube by a factor of two. Figure 4-2 shows an example of this operation for interpolation within a hypercube defined by a three dimensional table (which is defined by 8 original data values).
3. Continue to interpolate and "collapse" dimensions until only a single point remains. Figures 4-3 and 4-4 show this process schematically for a three dimensional table, resulting in a final interpolated value at the point (x_p, y_p, z_p) .

Note that RIP does not allow extrapolation in multi-dimensional tables (as this would be likely to lead to unintended, unrealistic values). The program will terminate with a fatal error message if extrapolation is attempted.

FIGURE 4-2
COLLAPSING THE X-DIMENSION
 ARGONNE/MODEL DEVELOPMENT/WA

ARGONNE/MODEL DEVELOPMENT/MA

FIGURE 4-4
COLLAPSING THE Z-DIMENSION
 ARGONNE/MODEL DEVELOPMENT/WA

4.3.6 Defining an Event Parameter

When the user selects [Edit Parameter Definition] for an event parameter, a window labeled "Edit Event" will appear:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Parameter Editing			
Identifier : VOLCAN		Parameter No. : 35 of 38	
Description: volcanism			
Parameter Type : Event			
(Annual probability : RATE2)			
Save Ti	EDIT EVENT		
Edit Pa	Annual Rate of Occurrence : RATE2 (1.0E-7)		
[Affect	Can Event Reoccur : Yes		
[Function of]-			
F1=Prev Param F2=Next Param F3=Add Param F4=Delete Param			
F5=Find Param F6=Print Summary F7=Display Dist. F8=Expected Value			
F9=Strategy F10=Bayesian update (Current update level=0)			

Enter a numeric constant or the name of a parameter in the "Annual Rate of Occurrence" field. This is the Poisson rate. Note that any event with a rate of occurrence less than 10^{-10} is ignored in the disruptive event module (even if pruning factors are used).

Enter "Yes" or "No" (using the <PgUp> and <PgDn> keys) in the field labeled "Can Event Reoccur". RIP assumes events behave as Poisson processes. If the event cannot reoccur, RIP will recognize only the first occurrence of the event.

Note that the RIP disruptive event component model only recognizes one event per timestep. That is, if the rate of occurrence is such that more than one event occurs per timestep, only a single event is actually simulated.

During a simulation, when an event parameter is used in a function (i.e., when it affects some other parameter), the value of the event parameter is a function of time, taking on one of two values: it is equal to one if the event has occurred during the *current timestep*; and it is equal to zero if the event has not occurred during the current timestep.

It is possible for the rate of occurrence to change with time (as a result of being specified directly as a function of a time, or as a consequence of another event). It is important for the user to understand how RIP simulates a time variable rate of occurrence. This is discussed in Section 5.5 of the RIP Theory and Capabilities Manual.

4.3.7 Coded Function Parameters

In some instances, the user may wish to define a parameter as a complex function which can not be readily implemented using the function editing features described in Section 4.3.2. For example, a parameter's value may be dependent on a very complex set of logic which would be

cumbersome to represent using nested IF, THEN statements in the function editor. At a more complex level, representation of a parameter may require a numerical solution. For example, parameters representing the pressures at specific locations in the geosphere may be complex functions of a number of other parameters (including pressures at adjacent locations) such that calculation of these parameters is only possible by using a numerical technique (e.g., the finite difference method).

In order to deal with such situations, RIP is designed such that the user can develop separate coded program modules (written in the C programming language) which can then be directly coupled with the main RIP algorithms. The outputs of such modules are referred to as *coded functions*, which can be thought of as just another type of parameter. Note that theoretically, this feature allows complex process level models to be directly coupled into the RIP probabilistic structure. Practically, however, the complexity of such coded functions is limited by the necessity for the model to be computationally efficient in order to facilitate Monte Carlo simulation.

The manner in which these parameters are specified and coupled to RIP is described below.

4.3.7.1 Programming Coded Functions

In order to define a coded function within RIP, it is first necessary to write the C module of which the coded function is an output, and couple it into the main RIP algorithms. This entails three programming steps:

- creation of the actual C module;
- specification within the RIP front-end of the name of the C module and the number of arguments; and
- Addition within the RIP back-end (in a single location) of the function call.

The latter two steps are straightforward, such that the only serious programming required is the C module itself. The details of these steps are discussed in Appendix E.

Note that the C module can have as many as 70 input and 30 output arguments. As mentioned above, the output arguments become parameters within RIP.

As will be discussed below, once the programming changes discussed above have been implemented, the user interface can be used to control when and with what arguments the module will be called during program execution.

4.3.7.2 Adding Coded Functions to the Parameter Database

Unlike other types of parameters, coded function parameters can not be defined from within the parameters unit. Instead they are defined within a special editing window referred to as the

"Family Database Editor". A *coded function family* is defined by a specified C module, a specified set of input arguments, and a unique set of output arguments (referred to as coded functions). Specifying coded functions using families allows the same C module to be used for different situations within a simulation. For example, it may be necessary to use a complex C module to compute several parameters for each of a number of RIP pathways. These pathway parameters would all be computed in the same way (using the same C module), but the input arguments (associated with each particular pathway) would differ. This could be accomplished by defining a different family for each pathway (all of which use the same C module).

The family database editor is invoked by hitting the <Alt>-<F> key combination. (Note that this key combination is not available from within the parameters unit):

```

[■]-----Repository Integration Program (Rev. 4.04 )-----
      General      PA Model      Strategy Model      Results
      User's Guide Tutorial
Available Memory 311108      file date: 08-14-95 15:35:21

[■]-----Family Database Editor-----
                                     Family 2 of 3
Family Name       : FAMB
Coded Module Name : CMINIT
Description       : initialization function

Is Family dependent on Time : No      Force it : No
Is Family dependent on Group : No

Define Input Arguments
D
Define Output Arguments
E

Family Dependencies
Function of       : FAMA
Affects          : FAMC

F1=Prev
F2=Next
F3=Add
F4=Del
  
```

The user can add additional families with the <F3> key. Families can be deleted with the <F4> key. The <F1> and <F2> keys can be used to move between defined families.

The specific input fields are discussed below:

Family Name: This is a six character identifier for the family. It is not a parameter name (and can never be referenced by other parameters).

C Module Name: This is the name of the C module which is used to compute the coded function parameter(s). This is an option field which allows the user to toggle between the available modules.

Description: This is a 60 character description for the family.

Is Family Dependent on Time: This field can not be edited. It is determined automatically based on the input arguments specified below. The family is time-dependent if it is a direct (or indirect) function of either TIME or TEMP (which varies with time). Time-dependent families are automatically recomputed at the beginning of every timestep.

Force it: Even if a family is not dependent on TIME or TEMP, the user may still want to ensure that the family is computed every timestep. The user can toggle between Yes and No.

Is Family Dependent on Group: This field can not be edited. It is determined automatically based on the input parameters specified below. The family is group-dependent if it is a direct (or indirect) function of a specified environmental factor defining waste package groups (e.g., CONTAC, TEMP). Group-dependent families are automatically recomputed for each waste package group.

Define Input Arguments: This field provides access to the following window for specifying the input parameters for the family:

Repository Integration Program (Rev. 4.04)

General PA Model Strategy Model Results

User's Guide Tutorial

Available Memory 311108 file date: 08-14-95 15:35:21

Family Database Editor Family 2 of 3

Family Name : FAMB

Coded Module Name : CMINIT

Description : INPUT Argument Editor Argument 1 of 1

Is Family depe Argument : D (N/A)

Is Family depe F1=Prev F2=Next F3=Add F4=Delete

Define Input Arguments

D

Define Output Arguments

E

Family Dependencies

Function of : FAMA

Affects : FAMC

F1=Prev
F2=Next
F3=Add
F4=Del

These are the input arguments for the C module. They can be existing parameters names (including previously defined coded functions) or constants. They must be listed in the same order that they are used in the argument list of the C module.

The user can add input arguments with the <F3> key. Arguments can be deleted with the <F4> key. The <F1> and <F2> keys can be used to moved between defined arguments.

Define Output Arguments: This field provides access to the following window for specifying the output parameters for the family:

Repository Integration Program (Rev. 4.04)

General
PA Model
Strategy Model
Results

User's Guide Tutorial

Available Memory 311108
file date: 08-14-95 15:35:21

Family Database Editor
Family 2 of 3

Family Name : FAMB
Coded Module Name : CMINIT
Description :

OUTPUT Argument Editor
Argument 1 of 1

Is Family depe Argument : E (N/A)

Is Family depe F1=Prev F2=Next F3=Add F4=Delete

Define Input Arguments
D
Define Output Arguments
E

Family Dependencies
Function of : FAMA
Affects : FAMC

F1=Prev
F2=Next
F3=Add
F4=Del

These are the output arguments for the C module. They must be listed in the same order that they are used in the argument list of the C module. The specified output arguments are automatically added to the parameter database and can be referenced by other functions (including other coded functions).

The user can add output arguments with the <F3> key. Arguments can be deleted with the <F4> key. The <F1> and <F2> keys can be used to moved between defined arguments.

As noted above, it is possible for one family to be a function of another family. For example, if one family (e.g., FAMA) had two output arguments (coded function parameters) called A and B, a second family (e.g., FAMB) could use A and/or B as input parameters. RIP would automatically ensure that FAMA is always computed prior to FAMB, since FAMB requires output from FAMA as input arguments. Such dependencies between families are automatically listed (and can not be edited) under "Family Dependencies" in the family database editor. In the example shown, the current family (FAMB) is dependent on output from FAMA and produces input for FAMC.

Once output arguments have been defined, they are automatically added to the parameter database, as shown below:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
<div> <div>Parameter Editing</div> <div> Identifier : D Description: output from FAMA Parameter Type : Coded (Output argument to Hard-coded procedure) Save Time History : No Edit Parameter Definition (Affects)- [Function of]-Not implemented for coded parameters </div> <div> Parameter No. : 10 of 38 </div> </div>			
<div> F1=Prev Param F2=Next Param F3=Add Param F4=Delete Param F5=Find Param F6=Print Summary F7=Display Dist. F8=Expected Value F9=Strategy F10=Bayesian update (Current update level=0) </div>			

Other than the description field, coded parameters can not be modified in any way from within the parameter database. The delete key, <F4>, and the "Edit Parameter Definition" access field are inactive. Hence, a coded function parameter can not be deleted directly from the parameter database. The only ways to delete a coded function parameter are 1) to delete the entire family in which it is defined; or 2) to delete it from the output argument list of its family.

In addition, for coded functions (and any parameters which are functions of coded functions), the <F7>, <F8>, <F9>, and <F10> keys are not active in the parameter editing window.

Note that families can not be accessed (using <Alt>-<F>) from within the parameters unit. Likewise, the parameters unit can not be accessed (using <Alt>-<P>) from within the families database editor.

4.3.7.3 Computation of Coded Functions During Simulation

Although the C module which is used to compute a coded function is only added to a single location in the back-end source code, it can be invoked at several different points within the simulation. As discussed above, the input parameters for the particular family determine when the coded functions are computed, as summarized below:

- If a family is independent of time and waste package group, and if none of the input parameters are modified by disruptive events, the coded functions for the family are computed only at the beginning of the simulation.
- Whenever the input parameters for a family are modified by a disruptive event, the coded functions for the family are recomputed.
- If a family is dependent on time (or the user forces it to be so), the coded functions of the family are recomputed every timestep.
- If a family is dependent on waste package group, the coded functions for the family are computed separately for each group.

4.3.7.4 Limitations of the Use of Coded Functions

Because coded functions are computed by a separate C module contained within the back-end program, there is a key limitation on their use which the user must be aware of. A coded function (or any parameter that references it) can never be referenced within the disruptive events component model (since disruptive event calculations are carried out by the front-end program).

4.4 Displaying Stochastic Parameters and Functions

When defining stochastic parameters, particularly complex ones, it is often useful to view the form of the distribution when in the process of defining it. RIP gives the user this capability.

There are two ways to display the distribution of a stochastic parameter: 1) by sampling the specified distribution; and 2) by showing the analytical function which describes the distribution. The first approach samples the distribution a specified number of times and uses this information to graph the distribution. The second approach plots the specified analytical solution rather than sampling the distribution. The first distribution approaches the second as the number of samples grows large. Stochastic parameters can be displayed in either manner. Stochastic functions can only be displayed by sampling.

To display the distribution of a stochastic parameter or a stochastic function (excluding stochastic coded functions), press <F7> while in the "Parameter Editing" window. For stochastic parameters (as opposed to stochastic functions), RIP will first prompt the user to indicate whether he/she wants to generate Monte Carlo results for display. The user should answer No to display the analytical function directly. If the user answers Yes (generate Monte Carlo results), RIP will prompt for the *number of realizations* to sample for plotting the distribution.

For stochastic functions, it is not possible to display the exact solution, and Monte Carlo sampling is automatically implied. In this case, RIP will skip the first question and immediately prompt the user for the desired number of realizations.

If a stochastic function is dependent on TIME or a near-field environmental factor, the values for TIME and WP Group specified in the GENERAL window are used when evaluating the function.

In either case (exact solution or Monte Carlo sampling), the following screen will then appear:

```

[■]-----Repository Integration Program (Rev. 4.04 )-----
      General      PA Model      Strategy Model      Results
[■]-----Parameter Editing-----
[■]-- F4=Targets/Plot ----- PARAMETER DISPLAY WINDOW -----

Plot Type      : CDF      ----- Plot Range -----      Data Range -----
X-axis         : Linear   1          11          1.128889      9.927321
Y-axis         : Linear   0          1           0           1
Grid           : Yes      Number of bins for PDF plots : 20
Title          : Results for parameter A1,      100 realizations
X-axis Title   : Parameter A1: log-uniform distribution

----- Percentiles of the Parameter's Distribution -----
0.001 : 1.128889      Statistics: Mean      : 5.400861
0.01  : 1.149447      S.D.          : 2.426391
0.05  : 1.501662      Skewness   : 0.0471
0.10  : 2.433069      Kurtosis   : 1.844416
0.25  : 3.263246
0.50  : 5.376611
0.75  : 7.534341
0.90  : 8.777224
0.95  : 9.125556
0.99  : 9.852854
0.999 : 9.927321

----- Targets -----
Cum. Prob.: 0.5      Value      : 5.376611
Value      : 5.376611 Cum. Prob.: 0.5
Prob. Dens.: 4.857892

-----
F1=Screen Plot F2=Hardcopy Plot F3=Print Results-Array F5=Print CDF

```

This window has two parts: the top half allows the user to specify the characteristics of the graphical display. The bottom half displays the percentiles of the parameter's distribution and the distribution's statistics. The function key <F4> toggles between the two halves.

The bottom half of the screen displays the cumulative distribution for the parameter of interest. Eleven probability values, ranging from 0.001 to 0.999 are displayed. While in the lower screen, the user can request (under "Targets") the parameter value corresponding to a specific probability or the probability corresponding to a specific parameter value. If a particular probability value cannot be computed due to the limited number of realizations, RIP will display N/A for that field in the statistics list. The probability at a given level can be calculated if:

$$(0.5 / \# \text{ of Realizations}) \geq \text{Probability Level}$$

Thus, to compute values at the .001 and .999 probability levels, 500 realizations are required. This rule applies whether or not confidence bounds have been selected under the <General> window. (For more information on confidence bounds, please refer to Appendix C of the RIP Theory and Capabilities Manual.)

The top half of the screen allows the user to modify the axes and specify the form of the graphical output.

The arrow (or <TAB> and <SHIFT>-<TAB>) keys can be used to move between fields. The following fields may be edited:

Plot type	toggle between CDF (cumulative distribution function), PDF (probability density function) and CCDF (complementary cumulative distribution function) using <PgDn> or <PgUp>
X Axis and Y axis	toggle to select linear or log scale using <PgDn> or <PgUp>
X-axis plot range	define X limits of plot
Y-axis plot range	define Y limits of plot

Grid	toggle to turn grid on or off using <PgDn> or <PgUp>
Number of bins	enter a value between 2 and 250
Title	enter title for plot
X-axis Title	enter label for X axis

The "Number of bins for PDF plots" determines how a PDF is computed. PDFs are plotted as histograms, and are computed by dividing the results into a number of equal-width bins. The accuracy of the estimated probability density decreases as the number of bins increases (because there are fewer results in any given bin). A small number of bins, however, may obscure details of the distribution form. RIP defines a default number (which can be changed by the user) based on the number of realizations.

Within this window, the following function keys are active:

F1	Screen Plot
F2	Hardcopy Plot
F3	Print Results Array
F5	Print CDF File

Press <F1> for a screen display of the CDF, PDF or CCDF in the format that you have defined. Confidence bounds will only be plotted if this option is selected in the <General> window. Confidence bounds are discussed in detail in Appendix C of the RIP Theory and Capabilities Manual.

As discussed in Section 2.4, several methods can be used to capture or print this screen directly. <F2> produces a hardcopy plot file of the distribution. The user is prompted for a file name. The current version of RIP accommodates the HPGL2 output format. After leaving the parameters program, the user can send the file created here to a printer or plot device or load it into a suitable software program.

<F3> produces an ASCII file listing of all of the realized values (note: this is only available if the results were realized, as opposed to being directly generated). The user is prompted for a filename. Hitting <ENTER> at this prompts sends the results to the screen. An example listing (based on just 20 realizations) is shown below.


```

RESULT OF MONTE CARLO REALIZATIONS FOR PARAMETER A1
The mean of the results is      0.999
The standard deviation is      0.095
The skewness is      -0.028
The kurtosis is      2.216
There were      20 realizations.
There are 20 in the results list.
The total weight of the results is      20.000
The list of results is as follows :
  1 Result value = 8.17886E-01 Weight = 0.050000 Count = 1 Cum = 0.025000
  2 Result value = 8.50039E-01 Weight = 0.050000 Count = 1 Cum = 0.075000
  3 Result value = 8.77698E-01 Weight = 0.050000 Count = 1 Cum = 0.125000
  4 Result value = 9.14439E-01 Weight = 0.050000 Count = 1 Cum = 0.175000
  5 Result value = 9.16986E-01 Weight = 0.050000 Count = 1 Cum = 0.225000
  6 Result value = 9.34282E-01 Weight = 0.050000 Count = 1 Cum = 0.275000
  7 Result value = 9.54153E-01 Weight = 0.050000 Count = 1 Cum = 0.325000
  8 Result value = 9.63200E-01 Weight = 0.050000 Count = 1 Cum = 0.375000
  9 Result value = 9.74961E-01 Weight = 0.050000 Count = 1 Cum = 0.425000
 10 Result value = 9.91772E-01 Weight = 0.050000 Count = 1 Cum = 0.475000
 11 Result value = 1.01032E+00 Weight = 0.050000 Count = 1 Cum = 0.525000
 12 Result value = 1.01628E+00 Weight = 0.050000 Count = 1 Cum = 0.575000
 13 Result value = 1.03271E+00 Weight = 0.050000 Count = 1 Cum = 0.625000
 14 Result value = 1.05157E+00 Weight = 0.050000 Count = 1 Cum = 0.675000
 15 Result value = 1.05364E+00 Weight = 0.050000 Count = 1 Cum = 0.725000
 16 Result value = 1.08122E+00 Weight = 0.050000 Count = 1 Cum = 0.775000
 17 Result value = 1.09893E+00 Weight = 0.050000 Count = 1 Cum = 0.825000
 18 Result value = 1.12325E+00 Weight = 0.050000 Count = 1 Cum = 0.875000
 19 Result value = 1.13715E+00 Weight = 0.050000 Count = 1 Cum = 0.925000
 20 Result value = 1.17623E+00 Weight = 0.050000 Count = 1 Cum = 0.975000

```

Note that it is possible for the number of results listed to be less than the number of realizations. This is because RIP combines results which are close together by adjusting the result's weight (the sum of the weights of the individual results always adds to 1). The "Count" column indicates the number of realizations which have been combined for any given result.

The <F5> key creates an ASCII file of the CDF. This file includes more points than shown in the bottom portion of the window (which only displays 11 points). This enables the user to import the file into other software packages (e.g., spreadsheets). The user is prompted for the ASCII filename.

4.5 Application of the Parameters Module

After experimenting with the parameters module, the user will come to realize that it can be quite useful and powerful as a stand alone tool (i.e., external to other portions of the RIP software) for examining the behavior of stochastic functions. That is, the user can build relatively complex parameters which are described as complex functions of other parameters (some of which may be stochastic), and propagate the uncertainty through a specified mathematical model. Hence, the user can define a stochastic model of a system and then examine its behavior.

For example, parameter A may be defined as a complex function of the stochastic parameters B, C, D, E and F (incorporating IF, THEN logic and complex mathematical functionalities). The parameters module allows the user (by selecting <F7>) to propagate the uncertainty

represented in the probability distributions defining B, C, D and F through the mathematical model specified by the user in order to determine the probability distribution of A.

This ability can be very useful to the user for examining intermediate results not explicitly output by the main RIP program in order to fully appreciate the implications of the input data set.

5. DATA ENTRY AND APPLICATION OF THE PERFORMANCE ASSESSMENT MODEL

In this chapter, we describe the details of data entry for the performance assessment model. As discussed in Section 3.2.1, the data input windows for the performance assessment model are accessed by selecting [PA Model] from the top level menu. Input for the PA model is subdivided into five categories: [Waste Package], [Pathways], [Events], [Dose/risk], and [Make Transfer File].

Before attempting to input data into RIP, it is necessary for the user to first formalize the conceptual model for the system. This entails describing the characteristics and expected behavior of the waste package, the near field environmental conditions expected at the repository, and the transport pathways through which radionuclides can migrate in the environment. Building and documenting such a conceptual model requires both knowledge pertaining to the particular system to be simulated, and a clear understanding of the capabilities and limitations of the RIP software.

Before entering data into RIP, the user should organize and carefully develop the conceptual model of the site. Having developed an appropriate conceptual model of the system to be simulated, the data representing that conceptual model can be entered into RIP.

Before describing the details of the input windows, however, it is necessary to describe the order in which data are entered for the performance assessment model. When editing an existing data input set, the user can move through the menu and input windows in any manner desired. When creating an input data set from scratch, data is generally entered by stepping sequentially through the menus and input windows. However, because of the interdependency of several of the input windows, there are several exceptions to this rule. The necessary steps for entering data into the performance model when starting from scratch are as follows:

- 1) Specify all input under [Pathways]
- 2) Specify input under [Waste Package] as follows:
 - a) Under [Near Field Conditions], specify input for [Water Contact Modes] and [Other Factors]. Do not specify input for [Temperature Conditions] at this time.
 - b) Under [Waste Package Description], specify all input, making sure to specify those inputs under the **Inventory** access field within the main waste package input window first.
 - c) Return to [Near Field Conditions], and specify input for [Temperature Conditions].
- 3) Specify all input under [Events].
- 4) Specify all input under [Dose/Risk].

5) Specify all data under [Make Transfer File], and create a transfer file for the back end.

Note that while entering data, the parameters module can be repeatedly accessed as described in the previous chapter in order to define any parameters specified in the input windows. The [General] input window can also be accessed in order to specify the graphics setup, save an echo file, change the species table, or modify the Monte Carlo sampling technique, as discussed in Section 3.4.

The various input windows under [PA Model] are described sequentially below.

5.1 Input for the Waste Package Behavior and Radionuclide Release Component Model

Selecting [Waste Package] from the menu under [PA Model] provides access to input windows for describing the waste package behavior and radionuclide release component model. Input for this component model is divided into three categories: [Near-Field Conditions], [Waste Package Description], and [Make WP Transfer File]. Each of these categories is discussed in detail below.

5.1.1 Describing Near-Field Conditions

Selecting [Near-Field Conditions] from the menu under [Waste Package] provides access to input windows for describing near-field conditions in the vicinity of the waste packages. Other waste package input parameters can subsequently be described in terms of these conditions. There are three categories of near-field conditions, each of which is represented by a menu item: [Water Contact Mode], [Temperature Conditions], and [Other Factors]. A fourth menu item, [Show Groups], is used to summarize the near-field conditions. Because the concepts involved in defining near-field conditions are somewhat complex and not self-explanatory, the discussion presented in this section is longer than those describing other aspects of the model.

Before discussing the details of specifying near-field conditions, it is necessary to understand how RIP enables the user to represent *variability* between waste packages. *Variability* should not be confused with *uncertainty*. Uncertainty in a model parameter implies a lack of knowledge regarding the actual value of the parameter. This is represented in RIP by describing the uncertain parameter as being stochastic (i.e., represented by a distribution). The parameter's distribution is sampled each realization. That single parameter value is then used throughout the realization. Variability in a model parameter, on the other hand, implies that for a given realization, a distribution of parameter values exist. Note that the variability that is represented here is a *random variability*. There are no spatial trends implied. The variability in a particular parameter occurs randomly throughout the repository.

Waste package-to-waste package variability is incorporated in the model by internally discretizing the waste package population into a discrete number of *waste package groups*. Groups are defined as a function of both near-field conditions and waste package type (e.g., spent fuel, defense waste). That is, a particular waste package group includes waste packages of a particular type which are subject to a specific set of near-field conditions. As will be discussed

in detail in Section 5.1.2, the user specifies the number of waste packages of each type that are emplaced in the repository. We describe here how waste package groups represent variable near-field conditions.

Near-field conditions are defined in terms of specified variable *environmental factors* (water contact mode, temperature, pH, redox conditions, stress, etc.). The user must determine which environmental factors he/she wishes to include in the model. Two environmental factors, water contact mode and temperature, are explicitly incorporated in the computational algorithm. As will be shown, the structure of RIP is such that other user-defined environmental factors can readily be added.

For each environmental factor that the user wishes to represent as being variable, it is necessary to define a distribution describing its variability. Based on additional user input (to be described below), RIP then converts the distribution describing the parameter's variability into an *equivalent discrete distribution*. (As will be discussed below, water contact mode is an exception to this rule: its variability is directly specified in a discrete manner.)

As an example, consider a case in which we assume that the environmental conditions can be defined in terms of only two controlling variable environmental factors: the mode of water contact and the temperature. To further simplify the example, assume that the variability distributions of these controlling parameters are already discretized. Since these parameters are described in terms of discrete distributions, they will automatically define a discrete number of *waste package groups*. For example, if we define water contact mode in terms of three discrete categories (e.g., "wet-drip", "moist-continuous" and "dry"), and temperature conditions in terms of three discrete categories (e.g., "hot", "warm", "cool"), the waste package population would be divided into $3 \times 3 = 9$ waste package groups. If more than one waste package type is included in a simulation (e.g., spent fuel and defense waste), the population would also be distinguished by waste package type, resulting effectively in $3 \times 3 \times 2 = 18$ groups. This is illustrated schematically in Figure 5-1.

A certain fraction of the entire waste package population will be located in each of these groups. For example, if 30% of the waste packages are "wet-drip", 20% of the waste packages are "warm", and 80% of the waste packages are of the type "spent fuel", then the "wet-drip", "warm", "spent fuel" waste package group would contain $(0.3 \times 0.2 \times 0.8 = 0.048)$ 4.8% of the waste packages.

(When computing the number of waste packages in each group, RIP rounds numbers to the nearest integer. Any deviation in the total number of waste packages is then corrected by adding or subtracting an appropriate number of waste packages to the largest group, while ensuring that the total number of packages of each type is preserved). Note that each group must have at least one waste package. If not, RIP will not allow a transfer file to be created and will produce an error message.

FIGURE 5-1
**EXAMPLE OF DISCRETIZATION OF REPOSITORY
 INTO WASTE PACKAGE GROUPS**
 ARGONNE/MODEL DEVELOPMENT

Each environmental factor has a name by which it can be referenced (e.g., CONTAC, TEMP, PH). Waste package parameters can be made dependent on environmental factors by referencing these names in a function. The value of these parameters would therefore vary from group to group. Within the computational algorithm, at every timestep within a realization RIP computes the release from each group, and then sums the results over all the groups to compute the total release from the repository.

Note that this representation of variability requires that the different environmental factors defined by the user be independent of each other. (e.g., the distribution of water contact modes is independent of the distribution of temperature). This and other aspects of RIP's representation of variability are discussed further in the RIP Theory and Capabilities Manual.

The actual manner in which environmental factors are specified is presented below.

5.1.1.1 Water Contact Mode

Selecting [Water Contact Mode] from the menu under [Near-Field Conditions] provides access to the following input window:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Near Field Conditions	Waste Package Description		Make WP File	
Water Contact Mode	Temperature Conditions	Other Factors	Show Groups	
Water Contact Mode				
Environmental factor ID : CONTAC	Value : 1	Mode 1 of 2	F1=Prev	
Water Contact Mode Description :	moist-continuous water contact			F2=Next
Fraction of Waste Packages Remaining : 1				F3=Add
Fraction remaining WPs in this mode : 0.4	(Constant)			F4=Del

Due to hydrogeologic variability, waste packages may be subject to different modes of water contact throughout the repository. This variability is represented in RIP by specifying a discrete distribution of *water contact modes* in the immediate vicinity of a waste package. The water contact modes are defined by the user. For an unsaturated repository, they might refer to local moisture conditions (e.g., dry, moist, dripping water), while for a saturated repository, they might refer to water velocity and the resulting mass transport modes which may be possible (e.g., zero velocity - diffusive transport only; high velocity - advective transport dominates). The water contact mode is referenced by the user by assigning an integer value to the internal environmental factor CONTAC, each integer value indicating (i.e., acting as an identifier for) a different water contact mode. Other processes and parameters can then be described as a function of water contact mode (e.g., mass transfer parameters and matrix alteration/dissolution processes). For example, if the user defined water contact modes A and B, with the integer identifiers 1 and 2, respectively, and then wanted a particular system parameter W to vary depending on the water contact mode, W could be defined as a function type parameter (see Section 4.3.2) using IF,THEN logic:

IF(CONTAC==1,50,100)

In this case, the parameter W would take on the value of 50 for contact mode A (CONTAC = 1), and the value of 100 for contact mode B.

For each value of CONTAC (i.e., for each water contact mode), the user must specify the fraction of waste packages subjected to those conditions. Hence, water contact mode is an exception to the rule described above which stated that the variability of the environmental factor is specified as a continuous distribution which is then converted to an equivalent discrete distribution. CONTAC is directly specified in a discrete manner.

In the example illustrated in Figure 5-1, "wet drip", "moist continuous" and "dry" refer to different values of CONTAC (e.g., 1, 2 and 3).

Note that water contact mode variability is assumed to be due to local random hydrogeologic conditions at the scale of the individual waste packages - it is not meant to represent large-scale spatial trends. In addition, note that the water contact mode represents the condition *after* the thermal period. As will be described below, waste packages may be defined such that they remain dry for some period of time due to a thermal pulse resulting from radioactive decay. The water contact modes, however, represent the expected conditions during the *post-thermal* period.

The function keys <F1> through <F4> can be used to add, delete or browse through the modes.

The specific inputs for this window are as follows:

Value: This is the integer identifier for a particular water contact mode. It can be specified by the user as any two digit integer value. Its default value is the mode number specified in the upper right hand corner of the input screen (i.e., for "Mode 2 of 4", Value is originally 2).

Water Contact Mode Description: This is a short description of the water contact mode, limited to 60 characters.

Fraction of remaining WPs in this mode: This is the *fraction of the remaining balance* of waste packages which are in this water contact mode. The "Fraction of Waste Packages Remaining" is specified in line immediately above this field. For example, suppose the user wished to define several contact modes. If the first was specified as having 40% of the waste packages, the window for the second water contact mode would look like this:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Near Field Conditions	Waste Package Description		Make WP File	
Water Contact Mode	Temperature Conditions	Other Factors	Show Groups	
Water Contact Mode				
Environmental factor ID : CONTAC	Value : 2	Mode 2 of 2	F1=Prev F2=Next F3=Add F4=Del	
Water Contact Mode Description :				
dry				
Fraction of Waste Packages Remaining : 0.6				
Fraction remaining WPs in this mode : 1			(Constant)	

RIP would indicate that 60% of the waste packages remain to be defined. Specifying 0.5 in the "fraction remaining" field would mean that 50% of the remaining packages (or 30% of the total) are allocated to water contact mode 2. The remaining 30% of the waste packages would have to be allocated to additional modes. Specifying 1 in this field would mean that all of the remaining waste packages (60% of the total) are in water contact mode 2.

For the last water contact mode defined, the value automatically takes on the value of 1. For other modes, however, this field can be specified as a parameter (a constant, a stochastic, or a function), with some constraints: It must *always* be greater than or equal to 0 and less than or equal to 1. Furthermore, if described as a function, the parameter *can not* be defined as a function of time or any environmental factor. Finally, the parameter cannot be (or cannot be a function of) a coded function.

Entering the *fraction of remaining balance* (as opposed to the *actual fraction*) may appear somewhat awkward. However, this convention allows the fractions to be represented stochastically, while still ensuring that they total to one. This convention is used in several other places within the RIP user interface and its proper application is discussed further in Appendix B.

A single water contact mode (implying no water contact mode variability) is the default.

Because the fraction of waste packages in each water contact mode can not vary with time, they can not directly respond to temporal changes in environmental conditions such as repository groundwater flux or temperature. Nevertheless, if this is deemed an important effect to consider, it can be accommodated in an approximate manner. As an illustrative example, suppose the user defines two water contact modes: mode A and mode B. Further suppose that under current repository flux conditions, the waste packages are split evenly between these two modes (50% in each). As the flux increases, however, more waste packages shift to mode B. This can be accommodated in an approximate manner by defining one or more *transition* modes. For illustrative purposes, we will denote mode AB as a transition mode. We might then say that modes A, AB, and B have 20%, 30%, and 50% of the waste packages, respectively. We can then define mode AB such that it is identical to mode A under low flux conditions (say $FLUX < 10$), and identical to mode B under high flux conditions ($FLUX > 10$). For example, if parameter W depends on the water contact mode (taking on the value of 50 in mode A and 100 in mode B), the user might specify W as follows:

$$W = \text{IF}(\text{CONTAC}==1, 50, W1)$$

where W1 and W2 are parameters defined as follows:

$$W1 = \text{IF}(\text{CONTAC}==2, 100, W2)$$

$$W2 = \text{IF}(\text{CONTAC}==3 \ \&\& \ \text{FLUX} \leq 10, 50, 100)$$

In this example, contact modes A, B and AB have been assigned the integer identifiers 1, 2, and 3, respectively. W would take on the value 50 if in contact mode A, 100 if in contact mode B, 50 if in contact mode AB and FLUX is less than or equal to 10, and 100 if in contact mode AB and FLUX is greater than 10. The transition could be made more continuous by defining additional transition modes (i.e., modes that switch behavior at intermediate flux values).

5.1.1.2 Temperature Conditions

Representation of temperature conditions at the waste package is described in detail in the RIP Theory and Capabilities Manual.

Selecting [Temperature Conditions] from the menu under [Near Field Conditions] provides access to input windows for describing temperature conditions.

The thermal behavior of the repository is represented in RIP by a built-in system parameter describing the temperature history at the edge of a waste package. This parameter is defined as a function of *waste package type*. Therefore, as discussed previously, temperature conditions can not be defined prior to defining the waste package types (which will be described below in Section 5.1.2). The temperature history is computed internally by RIP as follows:

$$\text{TEMPAV}_i(t) = T_m(t) + T_i(t) \quad (5.1)$$

where:

$\text{TEMPAV}_i(t)$ is the average temperature at the edge of waste package type i at time t;

$T_m(t)$ is the mean temperature in the host rock throughout the entire repository at time t;
and

$T_i(t)$ is the incremental temperature above the repository mean temperature at the edge of waste package type i at time t.

The user defines time histories for T_m and T_i as a series of discrete points, and specifies the uncertainties in these time histories. RIP interpolates between the specified points every 5 degrees. *That is, during a simulation, temperatures are updated in a stepwise fashion, whenever the temperature changes by more than 5 degrees.*

Because some of the controlling factors are likely to be variable, the actual temperature history at waste packages may vary significantly throughout the repository. This is represented in RIP by quantifying the *variability* about the average temperature $\text{TEMPAV}_i(t)$ and creating a *discrete*

distribution of temperature variability. The procedure, although straightforward, is not self-explanatory, and is detailed below.

Specification of temperature variability is carried out in two steps. First the user specifies the form of a variability distribution which is used to modify the average temperature $TEMPAV$. We refer to the variability parameter as $TEMPV$. In the current version of RIP, the distribution of this parameter can be either triangular or uniform, and must be symmetric about the value 1 (e.g., a uniform distribution between 0.85 and 1.15). Having specified the distribution, the user then specifies how this distribution is to be discretized by defining several (up to six) cumulative probability levels (e.g., 0.33, 0.66, 1.0). RIP then discretizes the distribution by using the expected value of the ranges defined by the specified probability levels as the discrete values. For example, specifying a uniform distribution with a variability of 15% (0.85 to 1.15), and discretization at the 0.33, 0.66, and 1.0 cumulative levels, defines the following discrete distribution:

<u>TEMPV</u>	<u>PROBABILITY</u>
0.9	0.33
1.0	0.33
1.1	0.34

The distribution has been discretized into three discrete values corresponding to the three ranges defined by the specified probability levels: 0 to 0.33, 0.33 to 0.66, and 0.66 to 1.0. The discrete values for the distribution are computed as the expected value of each range (e.g., the 0.333 cumulative probability level corresponds to a value of 0.95; the expected value of a uniform distribution between 0.85 and 0.95 is 0.9). Note that if a triangular distribution had been specified, the values would have been different, since the expected value in each range will be shifted toward 1.0.

The three discrete values described above would define three temperature categories that define variability across the repository: 33% of the packages would have a temperature of $0.9 \times TEMP_{AV_i}(t)$, 33% of the packages would have a temperature of $1.0 \times TEMP_{AV_i}(t)$, and 34% of the packages would have a temperature of $1.1 \times TEMP_{AV_i}(t)$.

A single value of $TEMPV$ of 1.0 (implying no variability in temperature) is the default for RIP.

The actual temperature at a particular waste package is referenced by the internal environmental factor $TEMP$ (which is completely analogous to the environmental factor $CONTAC$ discussed previously). Other waste package model parameters can subsequently be defined as a function of temperature, by referencing the name $TEMP$. At any given time, $TEMP$, as shown above, is computed internally by RIP as follows:

$$TEMP = TEMPV \times TEMP_{AV_i}(t) \quad (5.2)$$

In the example illustrated in Figure 5-1, "hot", "warm" and "cool" refer to different values of $TEMPV$ (e.g., 1.1, 1.0, 0.9). Hence, in this example, $TEMPV$ and $CONTAC$ are the environmental factors that define the waste package groups. Since $TEMPV$ varies between waste package groups, $TEMP$ also varies between waste package groups.

Having described the concepts behind the representation of temperature conditions in RIP, the manner in which the various temperature parameters are entered can be described. Selecting [Temperature Conditions] from the menu under [Near Field Conditions] provides access to the following input window:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Near Field Conditions	Waste Package Description		Make WP File	
Water Contact Mode	Temperature Conditions	Other Factors	Show Groups	
Temperature Conditions				
Repository mean temperature				
Incremental temperature at edge of WP				
Define temperature variability				
Rewetting temperature : REWET (78)				

The first two fields provide access to windows describing the mean temperature history in the rock (T_m) and the incremental temperature above the mean temperature at the edge of each type of waste package (T_i), respectively. The third field provides access to a window describing temperature variability throughout the repository. The fourth field is a parameter data field.

Repository Mean Temperature: This field provides access to the following input window for defining T_m :

Repository Integration Program (Rev. 4.04)				
General		PA Model		Results
User's Guide Tutorial				
Waste Package		Pathways	Events	Make Transfer File
Repository Mean Temperature				
Temperature Uncertainty		Time Uncertainty		
TMPUNC (1)		TIMUNC (1)		
Time (Yrs)	Temperature	Time (Yrs)	Temperature	
1 0	160	11 0	0	
2 100	150	12 0	0	
3 1000	100	13 0	0	
4 5000	75	14 0	0	
5 10000	60	15 0	0	
6 100000	30	16 0	0	
7 0	0	17 0	0	
8 0	0	18 0	0	
9 0	0	19 0	0	
10 0	0	20 0	0	

F1=Screen Display

Time/Temperature: These pairs must be entered as numbers (constants). RIP subsequently interpolates (linearly) in time between these pairs. The first and last points are interpolated horizontally. For example, if the first pair is specified as (time = 1000, temperature = 200), a temperature of 200 will be assigned to all times previous to time = 1000. Time is specified in years and must be non-negative. Temperature can be specified in any desired units. RIP allows up to 20 points.

Uncertainty in Temperature: This is used to specify the uncertainty in the temperature time history defined above. The user can specify this parameter as a constant, a stochastic, a table, or a function. The parameter can not, however, be specified as a function of time. Each realization, all of the inputs described above in the Temperature column are multiplied by the realized value of this parameter. *It is intended that the user specify this parameter as a stochastic centered about the value 1* (e.g., a triangular distribution centered at 1, with a minimum of 0.5 and a maximum of 2). This essentially shifts the temperature history up or down each realization, as illustrated schematically in Figure 5-2a. The user should be especially careful not to specify distributions that could result in unrealistic temperature histories.

Uncertainty in Time: This is also used to specify the uncertainty in the temperature time history defined above. The user can specify a parameter as a constant, a stochastic, or a function. The parameter can not, however, be specified as a function of time. Each realization, all of the inputs described above in the Time column are multiplied by the realized value of this parameter. *It is intended that the user specify this parameter as a stochastic centered about the value 1* (e.g., a triangular distribution centered at 1, with a minimum of 0.5 and a maximum of 2). This essentially shifts the temperature history left or right each realization, as illustrated schematically in Figure 5-2b. The user should be especially careful not to specify distributions that could result in unrealistic temperature histories.

The <F1> key plots (to the screen) the temperature history specified by the user. <Esc> erases the plot and returns the user to the input screen. <F2> creates a hardcopy plot (in HPGL2 format).

Incremental Temperature at Edge of WP: This field provides access to the following window for defining T_i :

```

[■] Repository Integration Program (Rev. 4.04 )
    General      PA Model      Strategy Model      Results
    User's Guide Tutorial

[■] Waste Package  Pathways  Events  Dose/Risk  Make Transfer File

[■] Incremental Temperature at edge of WP
    WP 1 of 1      WP ID : SPENT

    Temperature Uncertainty: WP1UN      (1      )

    Time (Yrs)  Temperature      Time (Yrs)  Temperature
    1 100      50      11 0      0
    2 1000     40      12 0      0
    3 5000     25      13 0      0
    4 10000    10      14 0      0
    5 100000   0       15 0      0
    6 0        0       16 0      0
    7 0        0       17 0      0
    8 0        0       18 0      0
    9 0        0       19 0      0
    10 0       0       20 0      0

    F1=Prev WP  F2=Next WP  F3=View Current  F4=View Current+Mean
  
```

FIGURE 5-2a
TEMPERATURE UNCERTAINTY
IN TIME/TEMPERATURE PAIRS
ARGONNE/MODEL DEVELOPMENT

FIGURE **5-2b**
TIME UNCERTAINTY IN
TIME/TEMPERATURE PAIRS
 ARGONNE/MODEL DEVELOPMENT

The user must specify an incremental temperature history for each waste package type that has been defined. Conversely, temperature histories can only be specified for waste package types that have previously been defined. The <F1> and <F2> keys are used to move back and forth through the different waste package types that have been defined.

Recall that the average temperature at the edge of a waste package type i is computed by RIP as $T_m(t) + T_i(t)$.

Time/Temperature: These pairs must be entered as numbers (constants). RIP subsequently interpolates (linearly) in time between these pairs. The first and last points are interpolated horizontally. For example, if the first pair is specified as (time = 1000, temperature = 200), a temperature of 200 will be assigned to all times previous to time = 1000. Time is specified in years and must be non-negative. Temperature can be specified in any desired units. RIP allows up to 20 pairs.

Uncertainty in Temperature: This is used to specify the uncertainty in the incremental temperature time history defined above. The user can specify a parameter as a constant, a stochastic, a table, or a function. The parameter can not, however, be specified as a function of time. Each realization, all of the inputs described above in the Temperature column are multiplied by the realized value of this parameter. It is intended that the user specify this parameter as a stochastic centered about the value 1 (e.g., a triangular distribution centered at 1, with a minimum of 0.5 and a maximum of 2). This essentially shifts the incremental temperature history up or down each realization. The user should be especially careful not to specify distributions that could result in unrealistic temperature histories.

Note that the user only specifies an uncertainty in the temperature and can not specify an uncertainty in time (with regard to the time/temperature pairs), as was done for the mean temperature in the rock.

The <F3> key provides a plot of the incremental temperature history just specified (T_i). <F4> provides a plot of the incremental temperature history plus the mean temperature history ($T_m + T_i$), showing the actual history of the average temperature at the waste package. Note that for a PC running DOS 5.0 (or above), screen plots can be sent directly to the printer by typing <Shift>-<PrintScreen>, as discussed in Section 2.4. <Esc> erases the plot and returns to the input screen.

Define Temperature Variability: This field provides access to the following window for defining temperature variability:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Near Field Conditions		Waste Package Description	Make WP File	
Water Contact Mode	Temperature Conditions	Other Factors	Show Groups	
Temperature Conditions				
Repository mean temperature				
Incremental temperature at edge of WP				
Define temperature variability				
Rewetting temperature : REWET (78)				
Define Temperature Variability				
Environmental Factor ID : TEMP				
Define type of variability : Uniform				
Define symmetric variability about 1 : 0.3				
Define Discretization Levels : 0.33 0.66 1				
0 0 0				

Define type of variability: This defines the type of distribution describing the temperature variability. The distribution can be either uniform or triangular, the user toggling between the two with the <PgUp> or <PgDn> keys.

Define symmetric variability about 1: This further defines the distribution representing the temperature variability. The uniform or triangular distribution is symmetric about 1. This particular field specifies the magnitude of the symmetric variability. For example, if a uniform distribution is specified, and a value of 0.3 is entered here, the uniform distribution defined would range from 0.7 to 1.3. This value must be specified as a number which is greater than or equal to 0 and less than or equal to 1. A value of 0 indicates no variability.

Define Discretization Levels: These are cumulative probability levels by which the continuous variability distribution defined directly above is to be converted to a discrete distribution. The manner in which this is done is described at the beginning of this section (5.1.1.2). These must be input as numbers which are greater than or equal to zero and less than or equal to 1. Because they are *cumulative* probability levels, they must increase from first to last (left to right). The first value must be non-zero, and the last specified value must be 1 (any remaining 0's after a 1 are ignored).

Rewetting Temperature: This is the temperature at which the waste packages rewet. It is only appropriate for repositories in which water can be driven away during a thermal period. For saturated repositories where this may not be possible, the rewetting temperature should be set to a large number (greater than the highest possible waste package temperature specified above so that the waste packages never dry out). It may be described as a constant, a stochastic or as a function (e.g., as a function of water contact mode, or repository level flux). It can not, however, be a function of time.

5.1.1.3 Other Factors

Selecting [Other Factors] from the menu under [Near Field Conditions] provides access to input windows for defining other environmental factors (e.g., pH, stress, redox conditions) whose

variability the user wishes to include in the model. The user first defines the name (ID) of the environmental factor (e.g., PH) and the average value about which the environmental factor's variability is to be centered (e.g., 7). Note that this average value need not be a constant, and may be described stochastically or as a function. A variability distribution is then defined in the same manner as described for temperature (e.g., 0.9, 1.0, 1.1). We refer to each of these discrete values in the distribution as the *variability factor* for each environmental factor category. In this example, we would refer to this factor as PH_V (that is, the environmental factor name with "_V" appended on to the end). PH_V is analogous to TEMPV discussed in Section 5.1.1.2. This would define a number of discrete PH categories (e.g., $0.9 \times 7 = 6.3$, $1.0 \times 7 = 7.0$, $1.1 \times 7 = 7.7$).

The user-defined environmental factor ID (in this case PH) is completely analogous to the internal environmental factors CONTAC and TEMP discussed previously. That is, other waste package parameters could subsequently be defined as a function of the pH, which would be variable through the repository, by referencing the environmental factor name PH. In the example illustrated in Figure 5-1, adding the three pH categories (e.g., "acidic" corresponding to 6.3, "neutral" corresponding to 7.0, and "basic" corresponding to 7.7) would add a fourth dimension to the diagram, resulting in $3 \times 3 \times 2 \times 3 = 54$ waste package groups. As shown above, the actual value of the environmental factor (in this case, the pH) at any time in any particular group is computed as the product of the average value of the factor and the variability factor. In this example,

$$PH = (\text{average value of pH}) \times PH_V$$

Because PH_V varies from group to group, PH (which can be referenced by the user) varies from group to group.

The following input window is accessed by selecting [Other Factors] from the menu under [Near Field Conditions]:

Repository Integration Program (Rev. 4.04)				
General	FA Model	Strategy Model	Results	
User's Guide Tutorial				
[]				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
[]				
Near Field Conditions	Waste Package Description		Make WP File	
[]				
Water Contact Mode	Temperature Conditions	Other Factors	Show Groups	
[]				
Environmental Factors				
Environmental Factor ID : PH		Factor 1 of 1		F1=Prev
Parameter : MEANPH (7)				F2=Next
Define type of variability : Uniform				F3=Add
Define symmetric variability about 1 : 0.1				F4=Del
Define Discretization Levels : 0.33		0.66	1	
0		0	0	

Environmental Factor ID: This is the name by which the environmental factor can be referenced by the user. It is limited to six characters.

Parameter: This is the parameter which defines the average value of the environmental factor about which the variability is to be defined. It can be specified as a constant, a stochastic, or a function.

Note that environmental factors cannot be defined recursively. For example, if PH and REDOX are defined as environmental factors, the average value for PH can be described as a function of REDOX *only if* the average value for REDOX is independent of PH.

Define type of variability: This defines the type of distribution describing the environmental factor's variability. The distribution can be either uniform or triangular, the user toggling between the two with the <PgUp> or <PgDn> keys.

Define symmetric variability about 1: This further defines the distribution representing the environmental factor's variability. The uniform or triangular distribution is symmetric about 1. This particular field specifies the magnitude of the symmetric variability. For example, if a uniform distribution is specified, and a value of 0.3 is entered here, the uniform distribution defined would range from 0.7 to 1.3. This value must be specified as a number that is greater than or equal to 0 and less than or equal to 1.

Define Discretization Levels: These are cumulative probability levels by which the continuous variability distribution defined directly above is to be converted to a discrete distribution. The manner in which this is done is identical to that for temperature variability, described at the beginning of Section 5.1.1.2. These must be input as numbers that are greater than or equal to zero and less than or equal to 1. Because they are *cumulative* probability levels, they must increase from first to last (left to right). The first value must be non-zero, and the last specified value must be 1 (any remaining 0's after a 1 are ignored).

The user can move through environmental factors that have been defined with the <F1> and <F2> keys. Environmental factors can be added or deleted with the <F3> and <F4> keys, respectively.

5.1.1.4 Show Groups

Selecting [Show Groups] from the menu under [Near Field Conditions] does not provide access to any input windows. Rather, it provides a summary display of all of the waste package groups that have been defined by the user. The display window appears as follows:

r[■] Repository Integration Program (Rev. 4.04)

Group #	# WPs	WP TYPE	CONTAC	TEMPV	PH_V
1	436	1	1	0.7990	0.9330
2	436	1	1	0.7990	0.9990
3	449	1	1	0.7990	1.0660
4	436	1	1	0.9970	0.9330
5	436	1	1	0.9970	0.9990
6	449	1	1	0.9970	1.0660
7	449	1	1	1.1980	0.9330
8	449	1	1	1.1980	0.9990
9	462	1	1	1.1980	1.0660
10	653	1	2	0.7990	0.9330
11	653	1	2	0.7990	0.9990
12	673	1	2	0.7990	1.0660
13	653	1	2	0.9970	0.9330
14	653	1	2	0.9970	0.9990
15	673	1	2	0.9970	1.0660
16	673	1	2	1.1980	0.9330
17	673	1	2	1.1980	0.9990
18	694	1	2	1.1980	1.0660

In this particular example, the user has defined (using the previous input windows) 1 waste package type, 3 water contact modes, 3 temperature categories, and 2 categories of the user-defined environmental factor PH. This results in $1 \times 3 \times 3 \times 2 = 18$ waste package groups.

For each group, the number of waste packages, the waste package type, the water contact mode (CONTAC), the temperature variability factor (TEMPV), and the variability factor for other user-defined environmental factors (in this case, PH_V) are displayed. For example, the screen shown above indicates that waste package group 1 has 436 waste packages of type 1 in water contact mode 1, with a temperature history 0.799 times the average temperature, and a pH 0.933 times the average pH.

Note that if groups are defined stochastically, the values shown by [Show Groups] are computed based on expected values of the stochastic inputs.

[Show Groups] is a useful option for summarizing and verifying the waste package-to-waste package variability that the user has specified.

5.1.2 Describing Waste Package Behavior and Radionuclide Release

Selecting [Waste Package Description] from the menu under [Waste Package] provides access to input windows for specifying the details of waste package behavior and radionuclide release. The following input window is displayed:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
Waste Package Database Editor			
ID : SPENT	Package 1	of 2	F1=Prev
DESC: Spend nuclear fuel			F2=Next
			F3=Add
			F4=Del
			F5=Copy
			F6=Copy
			Inventory
Number of Packages : 10000			
MTHM per Package : 1			
Waste Burnup (MWd/MTHM): 1			
Is mass transfer/bound exposure independent of failure mode? : No			
Mass Transfer			
Exposure			
Primary Container Failure Definition	Plotting Options		
Secondary Container Failure Definition	» Rewetting time : 0		
Inventory	» Cont. fail time : 0		
Define Discharge Pathways	Plot axes : automatic		
(AE,1.00)			
Output Selections			
Total Discharges : No	Discharges by RN : No		
Total Discharge Histories : No	Discharge Histories by RN : No		

The <F1> and <F2> keys can be used to move between defined waste package types. The user can add additional waste package types with the <F3> key. Waste package types can be deleted with the <F4> key. The <F5> key copies all the data for the current waste package to a new waste package. The <F6> key copies the inventory from another waste package into the current waste package.

Specification of multiple waste package types allows the user to represent the different kinds of waste packages that will be emplaced in the repository (e.g., spent fuel, high level defense waste). This is necessary because different kinds of waste packages may behave quite differently (e.g., each type having different inventories, container failure rates, and/or mass exposure and mass transfer characteristics).

Note that different waste package types could be defined to represent waste packages which are similar but behave slightly differently. For example, a waste package type could be defined that had slightly cooler temperatures to represent those waste packages which are emplaced near the edge of the repository.

The specific input fields in the waste package window shown above are discussed in the following sections.

5.1.2.1 Waste Package Characteristics

For each waste package type, the following input is required:

ID: This is a six character identifier for the waste package type.

DESC: This is a 60 character description for the waste package type.

Number of Packages: This is the number of waste packages of this particular type emplaced in the repository. This must be a non-negative integer.

MTHM per Package: This is the total mass of waste as MTHM (metric tons of heavy metal). It must be a positive constant. This input is only used in order to provide normalized releases per 40 CFR Part 191. If the user is not interested in this particular form of output, he/she can choose not to compute it (as discussed in Sections 5.1.3 and 5.4), and this input can be specified as any positive value. Appendix C discusses in detail how the normalization is carried out.

For spent fuel waste, this input is straightforward, as this is often the form in which the available data are reported. It can also be computed from the mass in kg by assuming that, for all practical purposes, the waste matrix consists of UO_2 , and using the stoichiometric ratio of UO_2 to U ($270/238 = 1.13$).

Waste Burnup (MWd/MTHM): This is the waste burnup in terms of MegaWatt-days/MTHM. It must be a positive constant. This input is also necessary in order to provide normalized releases per 40 CFR Part 191. If the user is not interested in this particular form of the output, he/she can choose not to compute it (as discussed in Sections 5.1.3 and 5.4), and this input can be specified as any positive value. Appendix C discusses in detail how the normalization is carried out.

When specifying a waste burnup for spent fuel, the user should make sure that the specified burnup is consistent with the radionuclide inventories specified elsewhere (since the inventories should vary with burnup).

Is mass transfer/bound exposure independent of failure mode?: This is an option field which can be selected as Yes or No. If answered as No, several of the input parameters describing mass transfer and bound exposure become dependent on the mode in which the waste package primary container failed (discussed in detail in Sections 3.2.3.3 and 3.2.4.1 of the RIP Theory and Capabilities Manual). If answered as Yes, all mass transfer and bound exposure parameters are independent of the mode of container failure. As will be detailed subsequently, this option field affects the appearance of several subsequent windows ("Mass Transfer", "Exposure", and "Primary Container Failure Definition").

5.1.2.2 Mass Transfer Parameters

Mass Transfer: This field provides access to an input window for describing mass transfer out of and away from the waste package. The user should refer to Section 3.2.4 of the RIP Theory and Capability Manual to review the manner in which mass transfer is represented in RIP.

In summary, mass transfer is represented in RIP by the following equations:

$$k_{tp}(n) = k_{tp,a}(n) + k_{tp,d}(n) \quad (5.3)$$

$$k_{tp,a}(n) = \text{FLOW} \times \text{CATCH} \times C(n) \quad (5.4)$$

$$k_{tp,d}(n) = D_{eff}(n) \times \omega \times C(n) \quad (5.5)$$

$$C(n) = \text{MIN}\left[\frac{M_p(n)}{V_w + K_d(n) M_s}, C_s(n)\right] \quad (5.6)$$

where:

- $k_{tp}(n)$ = maximum possible mass transfer rate (from a single waste package) for radionuclide n [g/yr];
- $k_{tp,a}(n)$ = maximum possible advective mass transfer rate (from a single package) for radionuclide n [g/yr];
- $k_{tp,d}(n)$ = maximum possible diffusive mass transfer rate (from a single package) for radionuclide n [g/yr];
- FLOW = repository level groundwater infiltration rate [m/yr];
- CATCH = effective catchment area for a waste package [m²];
- $D_{eff}(n)$ = effective diffusion coefficient for radionuclide n [m²/yr];
- ω = geometric factor for diffusive mass transfer [m];
- $C(n)$ = the effective concentration of radionuclide n at the waste package [g/m³];
- $C_s(n)$ = saturation concentration of radionuclide n [g/m³];
- V_w = volume of water in contact with waste matrix in a failed waste package [m³];
- M_s = mass of sorbent in the waste package [kg];
- $K_d(n)$ = equilibrium partition coefficient for radionuclide n [m³/kg]; and
- $M_p(n)$ = average exposed mass of radionuclide n per failed waste package (computed internally by RIP) [g].

As mentioned above, the specific input required varies depending on whether mass transfer is described as a function of container failure mode. If mass transfer is independent of failure mode, the following window is accessed by this field:

Repository Integration Program (Rev. 4.04)			
General		PA Model	Strategy Model
User's Guide Tutorial			
Waste Package Database Editor			
ID : HLDW	Package 2 of 2		F1=Prev
DESC: vitrified waste			F2=Next
Number of Packages : 10000			F3=Add
MT: ☐ MASS TRANSFER			F4=Del
Wa	Repository Flow Rate (m/yr): FLOW	(21.49758)	copy copy tory
Is	Effective Catchment Area (m ²): CATCH	(0.5)	
Ma	Geometric Factor for Diffusion (m): OMEGA	(0.001)	
Ex	Water Volume Contacting Matrix (m ³): 0.1	(Constant)	
Pr	Mass of Sorbent (kg): 1.3	(Constant)	
Se	Equilibrium Partition Coefficients		
In	Define Discharge Pathways (AE, 1.00)		
Output Selections			
Total Discharges : No	Discharges by RN : No		
Total Discharge Histories : No	Discharge Histories by RN : No		

Repository Flow Rate: This is the groundwater flow rate (in m/yr) at the repository level. It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative.

Effective Catchment Area: This is the effective catchment area (in m²) perpendicular to the direction of groundwater flow for one waste package. It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative. It is multiplied by the repository flow rate to compute the effective volume rate of flow of water which is at a concentration of C(n).

Geometric Factor for Diffusion: The geometric diffusion factor has units of length (m), and represents *steady-state* diffusive transport. It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative and cannot be a function of time. Specification of this parameter is discussed in more detail in the Theory and Capabilities Manual, Section 3.2.4.1.

Water Volume Contacting Matrix: This is the volume of water (in m³) in contact with waste matrix in a failed container. It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative. It is used to compute the effective concentration at a failed waste package for radionuclides which are not solubility controlled. It represents the volume of water which is at the effective concentration C(n). Specification of a very small value here is conservative in that it ensures that the effective concentration is equal to the saturation concentration.

Mass of Sorbent (kg): This is the mass of sorbent in the waste package which can act to "buffer" the concentration in the water within the waste package (see Section 3.2.4.1 of the RIP theory and Capabilities Manual). It should be specified in units of kg. It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative.

Equilibrium Partition Coefficients (m³/kg): This accounts for the fact that, even for highly soluble elements, not all of the radionuclide mass in a waste package will

necessarily be dissolved. Some of it may be sorbed onto solids within the waste package.

Pressing this field provides access to the following window for specifying the equilibrium partition coefficients:

Repository Integration Program (Rev. 4.04)			
General		PA Model	Strategy Model
User's Guide Tutorial			
Waste Package Database Editor			
ID : HLDW	Package 2 of 2	F1=Prev F2=Next F3=Add F4=Del	
DESC: vitrified waste			
Number of Packages : 10000			
MT [] MASS TRANSFER			
Wa	Ref [] Equilibrium Partition Coefficients	) copy	
Is	Eff	Group 1 of 1	) copy
Ma	Ge Partition Coefficient (m ³ /kg) : KD1	(0.1)	)
Ex	Wa F1=Prev F2=Next		)
Pr	Mass of Sorbent (kg): 1.3	(Constant)	)
Se	Equilibrium Partition Coefficients		
In			
Define Discharge Pathways (AE, 1.00)			
Output Selections			
Total Discharges : No		Discharges by RN : No	
Total Discharge Histories : No		Discharge Histories by RN : No	

As discussed in Section 5.1.2.5, every element in the inventory of the specified waste packages is assigned to a *chemical element group*. Each chemical element group is referenced by an integer. Currently, RIP allows the user to specify up to 40 chemical element groups. In this window the user specifies the equilibrium partition coefficient for each chemical element group. It should be specified in units of m³/kg and pertains to the sorbent present within the waste package. It can be described as a constant, a stochastic, a table, or a function. It should always be specified as non-negative.

If mass transfer/bound exposure is indicated to be described as a function of container failure mode, "Effective Catchment Area" and "Geometric Factor for Diffusion" are not included in this window, as they must be input separately for each container failure mode:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
Waste Package Database Editor			
ID : SPENT	Package 1 of 2	F1=Prev	
DESC: Spend nuclear fuel		F2=Next	
Number of Packages : 10000		F3=Add	
MT [■] MASS TRANSFER		F4=Del	
Wa Repository Flow Rate (m/yr): FLOW	(21.49758)	copy	
Is Water Volume Contacting Matrix (m*m*m): 0.1	(Constant)	copy	
Ma Mass of Sorbent (kg): 1.3	(Constant)	tory	
Ex Equilibrium Partition Coefficients			
Pr			
Secondary Container Failure Definition » Cont. fail time : 0			
Inventory	Plot axes : automatic		
Define Discharge Pathways (AE,1.00)			
Output Selections			
Total Discharges : No	Discharges by RN : No		
Total Discharge Histories : No	Discharge Histories by RN : No		

The user should note that RIP waste package component model currently only represents steady-state mass transfer processes. It does not represent transient effects. As detailed in Section 3.2.4.3 of the RIP Theory and Capabilities Manual, however, transient solutions for mass transfer from the waste packages can be represented by appropriate use of the pathways component model.

5.1.2.3 Parameters Describing Bound Exposure (Alteration/Dissolution of the Waste Matrix)

Exposure: This field provides access to an input window for describing exposure of the radionuclide inventory bound within the waste matrix. The user should refer to Section 3.2.3.3 of the RIP Theory and Capability Manual to review the manner in which bound exposure is represented in RIP.

In summary, bound exposure is defined by the following equations:

$$k_{a/d} = k_{wat} + k_{air} \quad (5.7)$$

$$k_{wat} = R_{dis} \times S \times f_w \quad (5.8)$$

where:

$k_{a/d}$ = total fractional rate of matrix alteration/dissolution [1/yr];

k_{wat} = fractional alteration/dissolution rate of matrix in water [1/yr];

k_{air} = fractional alteration rate of matrix in air [1/yr];

R_{dis} = aqueous matrix alteration/dissolution rate [g/m²/yr];

S = effective surface area of waste matrix in a failed container per unit mass [m²/g];

f_w = fraction of waste matrix surface area in a failed container which is wet.

As mentioned above, the specific input required varies depending on whether bound exposure is described as a function of container failure mode. If bound exposure is independent of failure mode, the following window is accessed by this field:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
Waste Package Database Editor			
ID : HLDW	Package 2 of 2	F1=Prev	
DESC: vitrified waste		F2=Next	
Number of Packages : 10000		F3=Add	
		F4=Del	
MT [■] EXPOSURE Wa Air Alteration Rate (1/yr): AIR (0.00001) Is Matrix Dissolution Rate (g/m ² /yr): DISS (5) Ma Surface Area of Matrix (m ² /g): 0.0001 (Constant) Ex Fraction of Waste Wetted (0<x<1): 0.1 (Constant) Pr			copy copy tory
Secondary Container Failure Definition » Cont. fail time : 0			
Inventory Plot axes : automatic			
Define Discharge Pathways (AE,1.00)			
Output Selections			
Total Discharges : No	Discharges by RN : No		
Total Discharge Histories : No	Discharge Histories by RN : No		

Air Alteration Rate: This is the fractional air alteration (oxidation) rate (in yrs⁻¹) for the waste matrix. As discussed in the Theory and Capabilities Manual, RIP allows the user to assume that air alteration can have the effect of exposing bound radionuclides by making them accessible due to a change in structure or a loss of integrity of the waste matrix. Under these conditions, the structure of the matrix is assumed to be altered to the extent that exposure of bound radionuclides is no longer limited by the matrix dissolution. That is, the bound inventory could be exposed via air oxidation of the matrix without having to dissolve the matrix. If this is not a valid mechanism, of course, this input should be set to zero. It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative.

Matrix Dissolution Rate: This is the aqueous alteration/dissolution rate for the waste matrix (in g/m²/yr). It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative.

Surface Area of Matrix: This is the surface area of matrix *per unit mass* (m²/g). It is multiplied by the "matrix dissolution rate" and the "fraction of waste wetted" to compute the fractional alteration/dissolution rate. It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative.

Fraction of Waste Wetted: This is the fraction of the surface area of waste in a failed container which is actually wetted. It can be described as a constant, a stochastic, or a function. Because it represents a *fraction*, it must be greater than or equal to zero and less than or equal to one.

If mass transfer/bound exposure is indicated to be described as a function of container failure mode, "Fraction of Waste Wetted" is not included in this window, as it must be input separately for each container failure mode:

Repository Integration Program (Rev. 4.04)			
General		PA Model	Strategy Model
User's Guide Tutorial			
Waste Package Database Editor		Package 1 of 2	
ID : SPENT	DESC: Spend nuclear fuel		F1=Prev F2=Next F3=Add F4=Del
Number of Packages	: 10000		
MT [■]	EXPOSURE		
Wa	Air Alteration Rate	(1/yr): AIR	(0.00001)
Is	Matrix Dissolution Rate	(g/m ² /yr): DISS	(5)
Ma	Surface Area of Matrix	(m ² /g): 0.001	(Constant)
Ex			
Primary Container Failure Definition		» Rewetting time : 0	
Secondary Container Failure Definition		» Cont. fail time : 0	
Inventory		Plot axes : automatic	
Define Discharge Pathways (AE,1.00)			
Output Selections			
Total Discharges : No		Discharges by RN : No	
Total Discharge Histories : No		Discharge Histories by RN : No	

5.1.2.4 Describing Waste Package Failure

Plotting Options: Several plotting options are presented on the lower right hand side of the waste package database editor screen. These all pertain to creating screen and hardcopy plots of the failure distributions. As will be discussed, these plots can be created from within the "Primary Container Failure Definition" and "Secondary Container Failure Distribution" windows.

Rewetting time: As will be discussed below, primary container failure modes can be conditioned on the time of rewetting. That is, if desired, they may not start until the waste package is rewet. Since the rewetting time may vary throughout the repository, in order to plot the primary container failure distribution, the user must specify a rewetting time upon which the plot can be based. This must be a non-negative number. Note that when plotting a log-uniform primary failure distribution, the rewetting time must be specified as nonzero.

Cont. fail time: As will be discussed below, secondary container failure modes can be conditioned on the time of primary container failure. That is, if desired, they may not start until the primary container has failed. Since the primary container failure time varies from container to container, in order to plot a single secondary failure distribution, the user must specify a primary container failure time upon which the plot can be based. This must be a non-negative number. Note that when plotting a log-uniform secondary failure distribution, the container failure time must be specified as nonzero.

Plot axes: For either a plot of the primary or secondary failure distributions, the plot axes can be manually or automatically specified. If manual is chosen, RIP will prompt the user for the maximum and minimum for both the x and the y axes.

Primary Container Failure Definition: This field provides access to an input window for describing the primary container failure distribution for the waste packages. The user should refer to Section 3.2.2 of the RIP Theory and Capability Manual to review the manner in which container failure is represented in RIP. As mentioned above, the specific input required varies depending on whether mass transfer/bound exposure is described as a function of container failure mode. If mass transfer/bound exposure is independent of failure mode, the following window is accessed by this field:

Repository Integration Program (Rev. 4.04)			
General		PA Model	Strategy Model
User's Guide Tutorial			
Waste Package Database Editor			
ID : SPENT		Package 1 of 2	F1=Prev
DESC: Spend nuclear fuel			F2=Next
			F3=Add
Primary Container Failure Definition			
Description : general corrosion			
Start when Rewet : No		Fail Mode 1 of 2	
If no, Start time : 0		(Constant) for WP# 1	F1=PREV
Probability : 1		(Constant) WP ID : SPENT	F2=NEXT
Aging Rate : 0.9		(Constant)	F3=ADD
Distribution Type : Weibull			F4=DEL
Define Failure Mode			F5=VIEW
			F6=HARD
(AE,1.00)			
Output Selections			
Total Discharges : No		Discharges by RN : No	
Total Discharge Histories : No		Discharge Histories by RN : No	

The user can define as many separate failure modes as desired, and these modes are then combined by RIP in an appropriate manner to produce the total failure distribution. The user can add additional failure modes with the <F3> key. Failure modes can be deleted with the <F4> key. The <F1> and <F2> keys can be used to move between defined modes. The <F5> and <F6> keys are used to view the total failure distribution and will be described in greater detail below.

Description: This is a 60 character description for the failure mode.

Start when Rewet: This is an option field with two choices: Yes and No. If the user specifies Yes, the failure mode does not start until the waste package is rewet (i.e., until the temperature at the edge of the waste package is less than or equal to the rewetting temperature). If the user specifies No, the failure mode will start at whatever time is specified in the following field.

If no, start time: This is the start time for the failure mode if the user specifies No above (it is ignored if the user specifies Yes above). This can be a constant, a stochastic, or a function. It must, however, be non-negative. Also, because it represents a time, it cannot be specified as a function of time. The default value is 0.

Probability: This represents the probability that a random waste package will be susceptible to this particular failure mode (i.e., the fraction of waste packages which are susceptible to this mode). It acts as a scaling factor for the failure distribution. This can be a constant, a stochastic, or a function. It must, however, be greater than or equal to zero and less than or equal to one. Furthermore, it can not be a function of time. The default value is one.

For most container failure modes, this parameter will have only one of two values: 1 or 0. In this sense, it acts as an "on/off" indicator for failure modes. This might be used, for example, if failure modes depended on variable environmental factors. For example, if the particular failure mode was only active under a certain water contact mode (identified by CONTAC = 1), and inactive in the others, the parameter could be specified as follows:

$$\text{IF}(\text{CONTAC} = 1, 1, 0)$$

That is, if CONTAC = 1, the probability = 1, else the probability = 0. As will be discussed below, the aging rate can also be used in this manner to control which failure modes are active.

In some cases, the user may wish to specify this parameter as a fraction (as opposed to 0 or 1). For example, if a certain percentage (say 0.01%) of the waste packages failed due to faulty emplacement and the user wished to represent this mode of failure by a separate distribution (as opposed to incorporating it into other failure mode distributions), he/she would assign a probability of 0.0001 to whatever distribution was defined.

Aging Rate: Whereas the probability described above has the effect of scaling the frequency axis (i.e., the y-axis) of the failure distribution, the aging rate has the effect of stretching and/or shrinking the time axis (i.e., the x-axis) of the failure distribution. This parameter can be a constant, a stochastic, or a function, and, as will be discussed below, it *can* vary with time. It must, however, be non-negative. The default value is 1. The aging rate is discussed in detail in Section 3.2.2.3 of the Theory and Capabilities Manual.

The aging rate allows failure distributions to respond directly to time-varying environmental conditions. For example, the aging rate could be specified to increase (or decrease) with changes in temperature, repository level infiltration, or some other user defined parameter or environmental factor (such as pH). It is easiest to illustrate the use and physical significance of this parameter by considering an example. Suppose that the aging rate for a certain mode was described such that above a certain temperature (120°), the container aged (i.e., failed) at twice the rate as under the standard temperature under which the failure distribution for the mode was defined. To accomplish this, the aging rate could be described in the parameters module as follows:

$$\text{IF}(\text{TEMP} > 120, 2, 1)$$

If the container was subjected to this elevated temperature for, say the first 1000 years, the *effective* age of the container (with respect to that failure mode) would then be computed as 2000 years, twice the actual age. Hence, if the original failure distribution was defined such that 25% of the containers failed within 1000 years, and 60% of the containers failed within 2000 years, the model would compute that under the elevated temperature conditions, 60% of the containers would fail within 1000 years.

Unlike the probability (discussed above), the aging rate can be described directly as a function of time or as a function of some other time-varying parameter (e.g., temperature, pH, infiltration rate). Also, because the aging rate can either shrink or stretch the time axis (whereas the probability can only shrink the probability axis), it can be greater than one. When it is greater than one, it acts to accelerate the failure rate (with respect to the original distribution); when it is less than one, it acts to decelerate the failure rate.

In addition to using the aging rate in the manner specified above, it can also be used as an "on/off" switch for the failure mode (in the exact same manner as the probability described above). This is because an aging rate of 0 freezes the time axis, effectively turning off the mode.

Distribution.Type: This specifies the form of the failure distribution. It is an option field with the following choices: Weibull, exponential, uniform, log-uniform, and degenerate. The mathematical forms of these distributions are discussed in detail in Appendix F of the Theory and Capabilities Manual.

Define Failure Mode: This field provides access to input windows for specifying the parameters which define the failure mode distribution specified above. Each distribution type has a different input window:

Repository Integration Program (Rev. 4.04)			
General		FA Model	Strategy Model
User's Guide Tutorial			
Waste Package Database Editor		Package 1 of 2	
ID : SPENT	DESC: Spend nuclear fuel		F1=Prev F2=Next F3=Add
Description	Weibull Failure Distribution		F1=PREV F2=NEXT F3=ADD F4=DEL F5=VIEW F6=HARD
Start when			
If no, Sta	Weibull slope (α) : 2.5	(Constant)	
Probabilit	$\approx$ Mean Lifetime ($\beta - \epsilon$) : 5000	(Constant)	
Aging Rate			
Distributi	F1=Change distribution F2=Display F3=Hardcopy		
Define Failure Mode			
(AE,1.00)			
Output Selections			
Total Discharges	: No	Discharges by RN	: No
Total Discharge Histories	: No	Discharge Histories by RN	: No

☐ Repository Integration Program (Rev. 4.04)		
☐ General	☐ PA Model	☐ Strategy Model
☐ User's Guide Tutorial		
☐ Waste Package Database Editor		
ID : SPENT DESC: Spend nuclear fuel	Package 1 of 2	F1=Prev F2=Next F3=Add
☐ Description: Exponential Failure Distribution Start when If no, Sta Probabilit Aging Rate Distribution Type : Exponential <u>Define Failure Mode</u>	Lambda (1/Yrs) : 0.0001 (Constant) F1=Change distribution F2=Display F3=Hardcopy	F1=PREV F2=NEXT F3=ADD F4=DEL F5=VIEW F6=HARD
(AE,1.00)		
Output Selections		
Total Discharges : No Discharges by RN : No Total Discharge Histories : No Discharge Histories by RN : No		

☐ Repository Integration Program (Rev. 4.04)		
☐ General	☐ PA Model	☐ Strategy Model
☐ User's Guide Tutorial		
☐ Waste Package Database Editor		
ID : SPENT DESC: Spend nuclear fuel	Package 1 of 2	F1=Prev F2=Next F3=Add
☐ Description: Uniform Failure Distribution Start when If no, Sta Probabilit Aging Rate Distribution Type : Uniform <u>Define Failure Mode</u>	Duration (Yrs) : 4000 (Constant) F1=Change distribution F2=Display F3=Hardcopy	F1=PREV F2=NEXT F3=ADD F4=DEL F5=VIEW F6=HARD
(AE,1.00)		
Output Selections		
Total Discharges : No Discharges by RN : No Total Discharge Histories : No Discharge Histories by RN : No		

☐ Repository Integration Program (Rev. 4.04)		
☐ General	☐ PA Model	☐ Strategy Model
☐ User's Guide Tutorial		
☐ Waste Package Database Editor		
ID : SPENT DESC: Spend nuclear fuel	Package 1 of 2	F1=Prev F2=Next F3=Add
☐ Description: Log Uniform Failure Distribution Start when If no, Sta Probabilit Aging Rate Distribution Type : Log Uniform <u>Define Failure Mode</u>	Duration (Yrs) : 1000 (Constant) F1=Change distribution F2=Display F3=Hardcopy	F1=PREV F2=NEXT F3=ADD F4=DEL F5=VIEW F6=HARD
(AE,1.00)		
Output Selections		
Total Discharges : No Discharges by RN : No Total Discharge Histories : No Discharge Histories by RN : No		

The Weibull requires two parameters, the Weibull slope and the mean lifetime. The exponential, uniform, and log-uniform are defined by single parameters. The degenerate (in which waste packages are failed instantaneously) requires no parameters (only the starting time). All parameters describing distributions can be specified as constants, stochastics, tables, or functions. The parameters must be non-negative, and can not be described as a function of time.

Note that for the log-uniform distribution, the specified start time must be greater than 0.

Note that three function keys are active in the windows displayed above. <F1> allows the user to change the distribution defined in the previous field while in this window. Upon exiting out of the window, the "Distribution Type" displayed will be updated. <F2> provides a screen plot of the distribution. <F3> provides a hardcopy plot (in HPGL2 format) of the distribution. In this case, the user is prompted for a filename. As was discussed above under "Plotting Options", the user must specify the rewetting time assumed for the plot, and the plot axes. Note that aging rates are not incorporated into plots of failure distributions.

Hitting <Esc> returns the user to the Primary Container Failure input window. We have previously discussed function keys <F1> through <F4>. <F5> and <F6> are used to plot *combined* failure distributions. RIP combines all of the defined modes in an appropriate manner and provides a screen plot or hardcopy plot of the combined distribution. For hardcopy plots (in HPGL2 format), the user is prompted for a filename.

As mentioned above, the specific input required for each primary container failure mode varies depending on whether mass transfer/bound exposure is described as a function of container failure mode. If mass transfer/bound exposure is *dependent* on failure mode, the following window is accessed by the "Primary Container Failure Definition" field:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
Waste Package Database Editor			
ID : SPENT	Package 1 of 2	F1=Prev F2=Next F3=Add	
DESC: Spend nuclear fuel			
Primary Container Failure Definition			
Description : general corrosion			
Start when Rewet : No	Fail Mode 1 of 2		
If no, Start time : 0	(Constant) for WP# 1		
Probability : 1	(Constant) WP ID : SPENT	F1=PREV F2=NEXT F3=ADD F4=DEL F5=VIEW F6=HARD	
Aging Rate : 0.9	(Constant)		
Distribution Type : Weibull			
Define Failure Mode			
Alteration/Dissolution/Mass Transfer			
(AE,1.00)			
Output Selections			
Total Discharges : No	Discharges by RN : No		
Total Discharge Histories : No	Discharge Histories by RN : No		

This is identical to the input window described above, with the exception of an additional access field: "Alteration/Dissolution/Mass Transfer".

Alteration/Dissolution/Mass Transfer: This field provides access to the following input window:

Repository Integration Program (Rev. 4.04)			
General		FA Model	Strategy Model
User's Guide Tutorial			
Waste Package Database Editor			
ID : SPENT	Package 1 of 2		F1=Prev
DESC: Spend nuclear fuel			F2=Next
			F3=Add
Primary Container Failure Definition			
De [■] ALTERATION/DISSOLUTION/MASS TRANSFER			
St	Effective Catchment Area	(m ²): CATCH	(0.5)
If	Geometric Factor for Diffusion	(m): OMEGA	(0.001)
Pr	Fraction of Waste Wetted	(0<x<1): 0.1	(Constant)
Ag			REV
Distribution Type : Weibull		DD	
Define Failure Mode		F4=DEL	
Alteration/Dissolution/Mass Transfer		F5=VIEW	
		F6=HARD	
(AE,1.00)			
Output Selections			
Total Discharges	: No	Discharges by RN	: No
Total Discharge Histories	: No	Discharge Histories by RN	: No

The "Effective Catchment Area", "Geometric Factor for Diffusion", and "Fraction of Waste Wetted" must be entered here for *this particular primary container failure mode*. These parameters were discussed above under *Mass Transfer* and *Exposure*, and have the same meaning, the only difference being that in this case they are a function of the mode of primary container failure, and hence must be specified separately for each primary container failure mode which is defined. The manner in which this information is used by RIP is discussed in detail in the RIP Theory and Capabilities Manual, Sections 3.2.3.3 and 3.2.4.1.

Secondary Container Failure Definition: This field provides access to an input window for describing the secondary container (e.g., cladding or pour canister) failure distribution for the waste packages. The user should refer to Section 3.2.2 of the RIP Theory and Capability Manual to review the manner in which container failure is represented in RIP. The following window is accessed by this field:

Repository Integration Program (Rev. 4.04)			
General		PA Model	Strategy Model
		Results	
User's Guide Tutorial			
Waste Package Database Editor			
ID : SPENT		Package 1 of 2	F1=Prev
DESC: Spend nuclear fuel			F2=Next
			F3=Add
Secondary Container Failure Definition			
Description : creep rupture of cladding			
Start when Container Fails : No		Fail Mode 1 of 1	
Start Time : 0	(Constant)	for WP# 1	F1=PREV
Probability : 1	(Constant)	WP ID : SPENT	F2=NEXT
Distribution Type : Exponential			F3=ADD
Define Failure Mode			F4=DEL
			F5=VIEW
			F6=HARD
(AE,1.00)			
Output Selections			
Total Discharges	: No	Discharges by RN	: No
Total Discharge Histories	: No	Discharge Histories by RN	: No

The user can define as many separate failure modes as desired, and these modes are then combined by RIP in an appropriate manner to produce the total failure distribution. The user can add additional failure modes with the <F3> key. Failure modes can be deleted with the <F4> key. The <F1> and <F2> keys can be used to move between defined modes. The <F5> and <F6> keys are used to view the total failure distribution and will be described in greater detail below.

Description: This is a 60 character description for the failure mode.

Start when Container Fails: This is an option field with two choices: Yes and No. If the user specifies Yes, the failure mode does not start until the primary waste package container fails. If the user specifies No, the failure mode will start at whatever time is specified in the following field.

If no, start time: This is the start time for the failure mode if the user specifies No above (it is ignored if the user specifies Yes above). This can be a constant, a stochastic, or a function. It must, however, be non-negative. Also, because it represents a time, it cannot be specified as a function of time. The default value is 0.

Probability: This represents the probability that the secondary waste package container will be susceptible to this particular failure mode (i.e., the fraction of waste packages that are susceptible to this mode). It acts as a scaling factor for the failure distribution. This can be a constant, a stochastic, or a function. It must, however, be between 0 and 1. Furthermore, *it can not be a function of time*. The default value is 1.

For most container failure modes, this parameter will have only one of two values: 1 or 0. In this sense, it acts as an "on/off" indicator for failure modes. This might be used if failure modes depended on local environmental conditions. For example, if the particular failure mode was only active under a certain water contact mode (identified by CONTAC = 1), and inactive in the others, the parameter could be specified as follows:

IF(CONTAC==1,1,0)

That is, if CONTAC = 1, the probability = 1, else the probability = 0. Unlike the primary container failure modes, secondary container failure modes *do not* have an aging rate which can also be used in this manner to control which failure modes are active.

In some cases, the user may wish to specify this parameter as a fraction (as opposed to 0 or 1). For example, if a certain percentage (say 0.01%) of the waste packages failed due to faulty emplacement (e.g., poor handling) and the user wished to represent this mode of failure by a separate distribution (as opposed to incorporating it into other failure mode distributions), he/she would assign a probability of 0.0001 to whatever distribution was defined.

Distribution Type: This specifies the form of the failure distribution. It is an option field with the following choices: Weibull, exponential, uniform, log-uniform, and degenerate. The mathematical forms of these distributions are discussed in detail in Appendix F of the Theory and Capabilities Manual.

Define Failure Mode: This field provides access to input windows for specifying the parameters that define the failure mode distribution specified above. Each distribution type has a different input window; the windows are identical to those described above for the primary container failure modes.

The Weibull distribution requires two parameters, the Weibull slope and the mean lifetime. The exponential, uniform, and log-uniform are defined by single parameters. The degenerate (in which waste packages are failed instantaneously) requires no parameters (only a starting time). All parameters describing distributions can be specified as constants, stochastics, tables, or functions. The parameters must be non-negative, and can not be described as a function of time.

Note that for the log-uniform distribution, the specified start time must be greater than 0.

Note that three function keys are active in the windows displayed above. <F1> allows the user to change the distribution defined in the previous field while in this window. Upon exiting out of the window, the "Distribution Type" displayed will be updated. <F2> provides a screen plot of the distribution. <F3> provides a hardcopy plot (in HPGL2 format) of the distribution. In this case, the user is prompted for a filename. As was discussed above, the user must specify the rewetting time assumed for the plot, and the plot axes.

Hitting <Esc> returns the user to the Secondary Container Failure input window. We have previously discussed function keys <F1> through <F4>. <F5> and <F6> are used to plot *combined* failure distributions. RIP combines the specified modes in an appropriate manner and provides a screen plot or hardcopy plot of the combined distribution. For hardcopy plots (in HPGL2 format), the user is prompted for a filename.

5.1.2.5 Describing Radionuclide and Elemental Properties

Inventory: This field provides access to a window for defining the characteristics of each radionuclide in the inventory of the waste package:

Repository Integration Program (Rev. 4..04)	
General	PA Model Strategy Model Results
User's Guide Tutorial	
Waste Package Database Editor	
ID : SPENT DESC: Spend nuclear fuel	Package 1 of 2 F1=Prev F2=Next F3=Add
Waste Package Inventory	
Radionuclide ID: AM241 Half-Life (Yrs): 432.3144 RN Inventory (Ci/Container) : 1	2 of 55 Daughter Product : NP237 (Constant) F1=Prev species F2=Next species F3=Copy to all F4=Load invent. from species file F5=grams/Curies
Inventory Distribution:	
Free Fraction : 1 Gap Fraction : 0 Bound Fraction : 1.0	(Constant) of 1.0 (Constant) of 0 of 0
Element Solubility (g/m*m*m) : 1	(Constant)
Effective Diffusion Coefficient (m ² /yr) : 1	(Constant)
Is Element Gaseous : No	
If Gaseous, Mass Transfer Rate away from WP (g/yr):0	(Constant)
Chemical Element Group : 1	
Copy chem grp Yes	

The actual radionuclides that can be considered are defined externally to the user interface in the ASCII species table file, discussed in Section 3.1.1.

Decay chains are entirely defined by the daughter products which are specified in this table. Note that RIP only allows a single daughter product to be defined for a given radionuclide (branching is not permitted), and that characteristics of that daughter must be defined within the table. Although a radionuclide can not be defined to have multiple daughters, it can have multiple parents.

Radionuclide ID's are restricted to 6 characters. Note that the radionuclide ID *must* be specified as the element abbreviation (e.g., AM, U, PU) followed by the mass number. The reason for this restriction is that solubilities (and several other properties) are defined by element, not by isotope. For example, specified saturation concentrations must be partitioned automatically by RIP among the defined isotopes of the given element. Hence, all isotopes of the same element must be similarly named in order for RIP to recognize them as such.

The user should be aware that RIP will only compute saturation concentration based on the isotopes which are specified in the species table. Isotopes which are not included in the table (e.g., non-radioactive isotopes) are not considered in the calculation. Not including a significant non-radioactive isotope results in computed saturation concentrations which are overestimated.

Referring to the input window above, note that RIP indicates how many radionuclides are included in the inventory. This is equal to the number of radionuclides specified in species table. The user can scroll through the radionuclides with the <F1> and <F2> keys. Several other function keys are available to facilitate data input.

The <F3> key provides the capability to copy the data pertaining to the current radionuclide to all the other radionuclides. Any differences can be edited manually.

<F4> allows the user to import inventory information directly from the species table. This feature will be discussed in detail in Section 5.1.2.5.1.

The <F5> key toggles the inventory display between Ci/container and g/container. The specific activity of the isotope is used for the conversion.

RIP also allows chemical element groups to be isotope-specific. The "Copy chem grp" field is used to define the chemical element groups. This feature is discussed in detail in Section 5.1.2.5.2.

Note that the Radionuclide ID, the half-life, and the daughter product are display fields only and can not be edited. The user can only add or delete radionuclides from the inventory by editing (or specifying a different) species table. As will be described below, however, some radionuclides can be effectively removed from the inventory by specifying a 0 inventory.

Radionuclide Inventory: This is the *initial* radionuclide inventory in Curies per waste package or grams per waste package (depending on the units selected using <F5>). Note that this should represent the inventory *at the time of closure*, since this is $\text{TIME} = 0$ for RIP. It can be specified as a stochastic or a constant. It must, however, be non-negative. Specifying this as zero will only eliminate this radionuclide from the waste package if it is not a daughter product of some other radionuclide (with a non-zero inventory).

Free Fraction: This is the fraction of the inventory which is located in what is referred to in RIP as the "free inventory": that part of the inventory which is instantaneously released upon primary container failure. It can be a constant, a stochastic, or a function, but it must be greater than or equal to zero and less than or equal to one, and can not vary with time.

Gap Fraction: This is the *fraction of the remaining inventory* (displayed immediately to the right) which is located in what is referred to in RIP as the "gap inventory": that part of the inventory which is instantaneously released upon secondary container failure in a waste package in which the primary container has also failed. It can be a constant, a stochastic, or a function, but it must be greater than or equal to zero and less than or equal to one, and can not vary with time. Note that the bound fraction cannot be edited, as it must be equal to one (i.e., anything not in the free or the gap inventory must be in the bound inventory). The free, gap and bound inventories are discussed in detail in the RIP Theory and Capabilities Manual, Section 3.2.3.

The following five input fields are *elemental properties* as opposed to radionuclide properties. Hence, for any given element, all isotopes of the element are forced to have identical values for these five input fields. For example, if a user enters a solubility for

AM241, it is automatically copied by the user interface to all other isotopes of the same element.

Element Solubility: This is the elemental solubility in g/m^3 . This can be a constant, a stochastic, or a function, but must be non-negative.

Effective Diffusion Coefficient: This is the effective diffusion coefficient (from the waste form to the beginning of the first pathway in m^2/year). It should include the effects of tortuosity on the molecular diffusion coefficient. It can be a constant, a stochastic or a function, but must be non-negative. The effective diffusion coefficient is discussed in detail in Section 3.2.4.1 of the RIP Theory and Capabilities Manual.

Is Element Gaseous: This is an option field which identifies those elements which can be transported out of the waste package in the gaseous state (e.g., ^{14}C). It must be answered Yes or No. Answering Yes to this field does not imply that the radionuclide travels in the far-field in a gaseous transport pathway. It only implies that it can leave the waste package as a gas.

If Gaseous, Mass Transfer Rate away from WP: This field is only active if the user specifies Yes in the previous field. It is the gaseous mass transfer rate away from a single waste package in g/year . Specifying this input as a large number (e.g., 10^{10}) effectively ensures that the release is always controlled by the rate of exposure (as opposed to the rate of mass transfer). It can be a constant, a stochastic, or a function, but must be non-negative.

Chemical Element Group: This specifies the "chemical element group" to which this particular element belongs. RIP currently allows the user to divide the elements in the inventory into as many as 40 groups, each of which is defined by different sorptive properties. All elements within a particular group have the same sorptive behavior. Chemical element groups are referenced in three places: 1) when defining partition coefficients in the waste package (Section 5.1.2.2); 2) when defining retardation factors for various flow modes within a geosphere transport pathway (Section 5.2.1.2); and 3) when defining partition coefficients within a biocell pathway (Section 5.2.2). The user should specify the chemical element group for each radionuclide before referencing them.

Note that, unless otherwise specified, the chemical element group for all isotopes of the same element is forced to be the same (see Section 5.1.5.2 below). Furthermore, if more than one waste package type is defined, the chemical element group for any particular isotope is forced to be the same in every waste package type.

This is an option field which allows the user to toggle between the numbers 1 to 40, which identify the chemical element group.

5.1.2.5.1 Importing Inventory Data from the Species Table

In the waste package inventory window, the (<F4>) key provides a mechanism for importing inventory data from the species table:

Repository Integration Program (Rev. 4.00)			
General	PA Model	Strategy Model	Results
Version 4.00 Features			
Waste Package Database Editor			
ID : WP1	Package 1 of 1		F1=Prev F2=Next F3=Add
DESC:			
Waste Package Inventory			
Radionuclide ID: AC227	1 of 55		F1=Prev species F2=Next species F3=Copy to all F4=Load invent. from species file F5=grams/Curies Copy chem grp Yes
Half-Life (Yrs): 21.77191	Daughter Product : -		
RN Inventory (Ci/Container) : 0	(Constant)		
Inventory Distribution:			
Free Fraction : 0	(Constant) of 1.0		
Gap Fraction : 0	(Constant) of 1		
Bound Fraction : 1.0	of 1		
Element Solubility (g/m*m*m) : 0	(Constant)		
Effective Diffusion Coefficient (m ² /yr) : 0	(Constant)		
Is Element Gaseous : No			
If Gaseous, Mass Transfer Rate away from WP (g/yr):0	(Constant)		
Chemical Element Group : 1			

Pressing <F4> will bring up a dialog box, which lists the headings for all of the "extra" user-defined columns in the species table:

Repository Integration Program (Rev. 4.00)			
General	PA Model	Strategy Model	Results
Version 4.00 Features			
Waste Package Database Editor			
ID : WP1	Package 1 of 1		F1=Prev F2=Next F3=Add
DESC:			
Waste Package Inventory			
Radionuclide ID: AC227	1 of 55		F1=Prev species
<div style="border: 1px solid black; padding: 5px;"> Enter number of the species-table extra data column to use to autoload all inventories for waste package WP1 1 : COL#1 2 : COL#2 Selection: </div>			
Chemical Element Group : 1			

RIP will list all of the available "extra" columns in the species table (i.e., any column with a header other than those identified in Section 3.1.1). By selecting one of these columns, the data values from the species table are copied into the interface for that waste package, overwriting any values that have been previously specified. Note, however, that any inventories that have been entered in the interface as parameters (as opposed to constants) are NOT overwritten (the user is warned of this during the import procedure).

5.1.2.5.2 Allowing Chemical Element Groups to be Isotope-Specific

Previous versions of RIP forced the chemical element group (which is used to assign Kd values and retardation factors) to be the same for all isotopes of an element. In some special situations, however, it may be desirable to allow the chemical element group to vary among isotopes of the same element. RIP allows the user to implement such an option. This is specified in the Inventory editing window as shown below:

Repository Integration Program (Rev. 4.00)			
General	PA Model	Strategy Model	Results
Version 4.00 Features			
Waste Package Database Editor			
ID : WP1	Package 1 of 1		F1=Prev F2=Next F3=Add
DESC:			
Waste Package Inventory			
Radionuclide ID: AC227		1 of 55	F1=Prev species F2=Next species F3=Copy to all F4=Load invent. F5=grams/Curies
Half-Life (Yrs): 21.77191		Daughter Product : -	
RN Inventory (Ci/Container) : 0		(Constant)	
Inventory Distribution:			
Free Fraction : 0	(Constant)	of 1.0	
Gap Fraction : 0	(Constant)	of 1	
Bound Fraction : 1.0		of 1	
Element Solubility (g/m*m*m) : 0	(Constant)		Copy chem grp Yes
Effective Diffusion Coefficient (m'/yr) : 0		(Constant)	
Is Element Gaseous : No			
If Gaseous, Mass Transfer Rate away from WP (g/yr):0		(Constant)	
Chemical Element Group : 1			

"Copy chem grp" is an option field. The default is "Yes", and this forces the chemical element group to be identical for all isotopes of the same element. Changing this to "No" allows the chemical element group to vary among isotopes of the same element. Note that even when this field is set to "No", if more than one waste package type is defined, the chemical element group for any particular isotope is forced to be the same in every waste package type.

5.1.2.6 Linking the Waste Package Release to the Far-Field Transport Pathways

Define Discharge Pathways: This field provides access to the following window for specifying the far-field transport pathways to which mass for this particular waste package type is distributed upon release:

Repository Integration Program (Rev. 4.04)							
From waste package: SPENT				Output Selection			
Discharge Pathway	Discharge Rule 1 of 1			Statistics		History	
	Fraction		Remaining	SUM	RNS	SUM	RNS
SATUR1	0.4	(Constant)	1	Yes	Yes	Yes	Yes
UNSAT1	0.5	(Constant)	0.6	No	Yes	No	No
AE	1	(Constant)	0.3	Yes	No	Yes	No
N/A	()	()					
	()	()					
	()	()					
Species following this rule : All							
AC227 AM241 AM242 AM242M AM243 C14 CA41 CL36 CM243 CM244 CM245 CM246 CO60							
CS135 CS137 H3 I129 MO93 NB-S1 NB93 NB94 NI-S1 NI59 NI63 NP236 NP237 PA231							
PB210 PD107 PU238 PU239 PU240 PU241 PU242 RA226 RA228 SE-S1 SE79 SM1...more							
F1=Prev F2=Next F3=Add F4=Delete F5=Copy							

Discharge pathways are specified in terms of *discharge rules*. A discharge rule is a set of discharge pathways that is applicable to a particular set of radionuclides. A discharge rule, however, can only be partitioned to pathways which have been previously defined. Hence, the user must define the pathways within the main [Pathways] input window before specifying the release rules here. The user can add and delete rules using the <F3> and <F4> keys, respectively. The <F1> and <F2> keys are used to move forward and backward among the defined rules.

The window will display all of the defined discharge pathways for the current rule, with the last entry being "N/A". To add an additional discharge pathway, place the cursor on "N/A". This is an option field, with the options being all of the available pathways (and the AE). After specifying the pathway ID, the user enters the fraction of the remaining balance which is allocated to this pathway. The remaining balance is indicated immediately to the right of the field.

For the last discharge pathway defined, the value automatically takes on the value of 1. For other pathways, however, this field can be specified as a parameter (a constant, a stochastic, a table, or a function), with the constraint that it must *always* be greater than or equal to 0 and less than or equal to 1. Note that a total of nine discharge pathways can be specified for a given rule.

In the window shown above, mass is released to three separate discharge pathways: SATUR1, UNSAT1 and AE. In this example, 40% of the mass is assumed to be released to the first pathway, SATUR1, leaving 60% of the mass remaining to be partitioned. Specifying 0.5 as the fraction released into the second pathway, UNSAT1, means that 50% of the remaining balance (or 30% of the total) is partitioned to this pathway. The remaining 30% of the mass would be allocated to the third discharge pathway, AE. Specifying 1 in the fraction field means that all of the remaining mass (30% of the total) is released to this pathway. In other words, to calculate the fraction of total mass that is released to a particular pathway, multiply the value in the fraction field (e.g., 0.5) by the value in the remaining field (e.g., 0.6) to obtain the result (e.g., 0.3).

Entering the *fraction of remaining balance* (as opposed to the *actual fraction*) may appear somewhat awkward. However, this convention allows the fractions to be represented stochastically, while still ensuring that they total to one. This convention is used in several other places within the RIP user interface and its application is discussed further in Appendix B.

RIP automatically defines a special discharge location called AE, to which mass may discharge. This refers to the "accessible environment". The accessible environment can be assigned any meaning desired by the user, but is typically used to represent a regulatory boundary (e.g., the ground surface; some specified distance from the site).

For each defined rule, the user specifies whether All, Some or None of the radionuclides follow the rule. If only one rule has been defined, this is forced to All. When a new rule is added, the default value is None. To add radionuclides to a rule, move the cursor to this field and hit <ENTER>. This brings up a drop-down menu listing all radionuclides. The user marks (i.e., selects) or unmarks radionuclides by hitting <ENTER> when the cursor is on that radionuclide. The arrow keys are used to move up and down through the list. The <F1> key can be used to mark or unmark all radionuclides. Hitting <ESC> exits the list with the new entries.

The only way to delete a radionuclide from a rule is to add it to another rule (i.e., whenever a radionuclide is added to a rule, it is automatically deleted from the other rule). Note that in order to delete a rule, the user must first reassign all of the radionuclides associated with that rule (rules can only be deleted if they have no radionuclides associated with them).

The <F5> key copies all of the rules from another waste package or pathway (as will be discussed in Section 5.2.1.1, discharge rules for pathways are defined in an identical manner). The user is prompted for the ID of the waste package or pathway from which the rules are to be copied. Note that all of the existing rules are replaced when the new rules are copied.

The right side of the window described above is used to specify output options and is discussed below.

5.1.2.7 Saving Waste Package Release Outputs

RIP allows three categories of waste package release outputs to be saved:

- releases *from* each waste package group;
- releases *from* each waste package group *to* a particular pathway or the AE; and
- total (combined) releases from all waste packages.

The first two categories of output are specified in the Waste Package windows and are discussed below. The last category of output is specified just prior to creation of the transfer file, and is discussed in Section 5.5.

Note that with regard to the discussion below, when outputs are selected from the menu of a particular waste package *type* (e.g., spent nuclear fuel), RIP saves the releases from all waste package *groups* which include that particular type. (If no environmental variability is defined, *type* and *group* are synonymous).

Release from the waste package groups that include the current waste package type is saved using the Output Selection fields at the bottom of the Waste Package Database Editor menu, reproduced below:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
Waste Package Database Editor			
ID : SPENT	Package 1 of 2		F1=Prev
DESC: Spend nuclear fuel			F2=Next
Number of Packages : 10000			F3=Add
MTHM per Package : 1			F4=Del
Waste Burnup (Mwd/MTHM): 1			F5=Copy
Is mass transfer/bound exposure independent of failure mode? : No			F6=Copy
Mass Transfer			Inventory
Exposure			
Primary Container Failure Definition	» Rewetting time : 0		
Secondary Container Failure Definition	» Cont. fail time : 0		
Inventory	Plot axes : automatic		
Define Discharge Pathways			
(AE,1.00)			
Output Selections			
Total Discharges : No	Discharges by RN : No		
Total Discharge Histories : No	Discharge Histories by RN : No		

Four options are available:

- Selecting Yes for "Total Discharges" saves the cumulative release for all waste package groups which include this type summed over all radionuclides.
- Selecting Yes for "Total Discharge Histories" saves the time history of release for all waste package groups which include this type summed over all radionuclides. RIP saves histories for the five realizations with the highest cumulative normalized releases under 40 CFR 191.13.
- Selecting Yes for "Discharges by RN" saves the cumulative release for all waste package groups that include this type by radionuclide.
- Selecting Yes for "Discharge Histories by RN" saves the time history of release for all waste package groups that include this type by radionuclide.

As discussed in the following section, and in Section 5.5, the radionuclides for which results are saved are selected in the Main Output Selection window.

Releases from a particular waste package to a particular discharge pathway can be saved from within the Waste Package Discharge Window, shown below:

Repository Integration Program (Rev. 4.04)

From waste package: SPENT				Output Selection			
Discharge Pathway	Discharge Rule 1 of 1			Statistics		History	
	Fraction		Remaining	SUM	RNS	SUM	RNS
SATUR1	0.4	(Constant)	1	Yes	Yes	Yes	Yes
UNSAT1	0.5	(Constant)	0.6	No	Yes	No	No
AE	1	(Constant)	0.3	Yes	No	Yes	No
N/A	(	)					
	(	)					
	(	)					

Species following this rule : All
 AC227 AM241 AM242 AM242M AM243 C14 CA41 CL36 CM243 CM244 CM245 CM246 CO60
 CS135 CS137 H3 I129 MO93 NB-S1 NB93 NB94 NI-S1 NI59 NI63 NP236 NP237 PA231
 PB210 PD107 PU238 PU239 PU240 PU241 PU242 RA226 RA228 SE-S1 SE79 SM1...more

F1=Prev F2=Next F3=Add F4=Delete F5=Copy

The right side of this window is used to specify output. For any given discharge pathway, there are four options:

- Selecting Yes under "Statistics" and "Sum" saves the cumulative release from all waste package groups which include this type to the specified discharge pathway summed over all radionuclides.
- Selecting Yes under "History" and "Sum" and "saves the time history of release from all waste package groups which include this type to the specified discharge pathway summed over all radionuclides. RIP saves histories for the five realizations with the highest cumulative normalized releases under 40 CFR 191.13.
- Selecting Yes under "Statistics" and "RNs" saves the cumulative release from all waste package groups that include this type to the specified discharge pathway by radionuclide.
- Selecting Yes under "History" and "RNs" saves the time history of release from all waste package groups that include this type to the specified discharge pathway by radionuclide.

As discussed in Section 5.5, the radionuclides for which results are saved are selected in the Main Output Selection window.

5.1.3 Making a Waste Package Transfer File

RIP allows the user an option to simulate waste package behavior and radionuclide release independent from the radionuclide transport pathways. That is, if desired, the user can model just the release from the waste packages without considering the subsequent transport of the radionuclides to the accessible environment. To do this, the user creates a waste package

transfer file which contains only information pertaining to the waste package behavior and instructs the back end to only simulate radionuclide release from the waste packages.

If this option is selected, RIP essentially bypasses the pathways and dose/risk component models. All other aspects of the model, including any specified disruptive events, are still simulated (although, as discussed in Section 5.3.3, one particular event consequence, moving waste packages to a pathway, is not simulated when the pathways component model is bypassed).

Selecting [Make WP Transfer File] from the menu under [Waste Package] provides access to the input windows for specifying general information regarding the creation of a waste package transfer file. Having done so, the user can then create the transfer file from this window.

The input window is as follows:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Near Field Conditions	Waste Package Description		Make WP File	
<div> <div>WASTE PACKAGE MODEL</div> <div> Number of timesteps : 100 Length of timestep (yrs) : 100 Number of realizations : 1000 Run using expected values : No Select Desired Output Define Realization Classes Make WP binary Transfer File </div> </div>				

Number of timesteps: This is the number of timesteps to be simulated. It must be greater than or equal to one. The beginning of the simulation (time = 0) is defined as the time of closure.

Length of timestep: This is the timestep length in years. It must be non-negative.

Number of realizations: This is the number of Monte Carlo realizations to be simulated. It must be greater than or equal to one.

Run using expected values: This is an option field which is answered Yes or No. If Yes, a single realization using the expected value for all stochastic parameters is produced (and the previous input specifying the number of realizations is ignored). Note that this realization is generally close to the median realization, which is generally lower than the mean realization (since the mean is strongly affected by extreme realizations).

Select Desired Output: This provides access to an input window for defining the form of the output:

Repository Integration Program (Rev. 402A)

SELECT DESIRED OUTPUTS

Waste Pkg. Rel. rate 10 CFR 60.113 : No		Normalize by Table 1 No
--	--	----------------------------

Standard Outputs	Statistics		Time History	
	Sum	by RN	Sum	by RN
Total Release from all Waste Packages	Yes	No	Yes	No
Release from each Waste Package	AsIs	AsIs	AsIs	AsIs

Selected Waste Packages
 Selected Parameter Histories

Selected WP Histories

Select Species : All AC227 AM241 AM242 AM242M AM243 C14 CA41..

The user has a choice of the exact outputs which are to be saved in the results file. Note that choosing all of the available outputs could create very large output files.

The top portion of the window is used to select regulatory output.

Waste Pkg. Rel. rate (10 CFR 60.113): This saves the maximum annual radionuclide release rate (normalized to the 10 CFR 60.113 limit) achieved by any radionuclide over the length of the realization. Normalization of results is discussed in detail in Appendix C. For each realization, the single maximum annual release value and the ID of the radionuclide having the maximum annual release are saved. In addition, RIP also saves three other values for each realization: the time at which the maximum release occurred, the fraction of primary containers which have failed by 300 years, and the fraction of primary containers which have failed by 1000 years (these latter two can be used to evaluate "substantially complete containment").

Normalize by Table 1: This determines whether or not the two cumulative radionuclide release results described below are to be normalized. It does not pertain to the "Waste Package Release Rate" described above. If the user selects Yes, the cumulative releases below are normalized to the 40 CFR 191.13 limit (normalization is discussed in detail in Appendix C). If the user selects No, results are output in units of Curies.

Two types of "Standard Outputs" are available: Statistics and Time History data. The results in the Statistics column refer to results that are summed over all timesteps. That is, they are cumulative with respect to time. "Sum" indicates that results are summed over all radionuclides, while "by RN" indicates that a separate cumulative release is to be saved for each specified radionuclide. Results under the Time History column are saved at each timestep. "Sum" indicates that results are summed over all radionuclides, while "by RN" indicates that a separate set of release data is to be saved for each specified radionuclide. If

"by RN" is selected, only those radionuclides chosen in the "Select Species" window at the bottom of the screen will be saved.

For each category for which time history data is selected, time histories are saved only for those realizations that contain the five highest cumulative normalized releases (40 CFR 191.13).

Total Release From all Waste Packages: This saves the cumulative waste package release summed over all waste package groups, and can be saved at each time step and/or summed over the entire realization. If "Sum" is selected the cumulative waste package release (summed over all radionuclides) is saved for each realization. If "by RN" is selected the cumulative waste package release for each individual specified radionuclide is saved on each realization. Hitting <ENTER> on the field will bring up a pull-down menu with the choices "Yes" and "No". The arrow keys can be used to select the desired option.

Release From each Waste Package: This saves the cumulative waste package release for each waste package group, and can be saved at each time step and/or summed over the entire realization. If "Sum" is selected the cumulative waste package release (summed over all radionuclides) is saved for each realization. If "by RN" is selected the cumulative waste package release for each individual specified radionuclide is saved for each realization. This line serves as a global override for options specified in the individual waste package windows. Note that this does not include "From-To" type results (e.g., "from waste package A to pathway B"). Hitting <ENTER> on the field will bring up a pull-down menu with the choices "On", "Off", or "AsIs".

The arrow keys can be used to select the desired option. "AsIs", which is the default, saves results only for those items specified in the individual Waste Package windows. If "On" is selected, all results are saved for the specified option, while if "Off" is selected, none of the results are selected for the specified option, regardless of the settings in the Waste Package menu.

The next section provides access to windows which summarize all of the output selection options which were specified in other windows. Selecting a field (e.g., "Selected Waste Packages") accesses a window which summarizes all of the output options selected in the other windows (e.g., the Waste Package and Define Discharge Pathways windows):

Repository Integration Program (Rev. 4.04)

SELECT DESIRED OUTPUTS

Waste Pkg. Rel. rate 10 CFR 60.113 : No	Normalize by Table 1 No
--	----------------------------

Discharge from Waste Packages:
Total discharge from SPENT
Total discharge from SPENT to AE
Discharge by RN from HLDW

Selected Waste Packages Selected Parameter Histories	Selected WP Histories
---	-----------------------

Select Species : All AC227 AM241 AM242 AM242M AM243 C14 CA41..

Finally, the "Select Species" key is used to choose those radionuclides for which results are to be saved for all options which have been specified as "by RN". The two available options are "All" and "Some". Placing the cursor to this field and hitting <ENTER> brings up a drop-down menu listing all radionuclides:

Repository Integration Program (Rev. 4.04)

SELECT DESIRED OUTPUTS

Waste Pkg. Rel. rate 10 CFR 60.113 : No	Normalize by Table 1 No
--	----------------------------

Standard Outputs	Statistics		Time History	
	Sum	by RN	Sum	by RN
Total Release from all Waste Packages	Yes	No	Yes	No
Release from each	AsIs	AsIs	AsIs	AsIs

Selected Waste Pa
Selected Paramete

Select Species :

AC227
√AM241
√AM242
√AM242M
√AM243
C14
√CA41
√CL36
√CM243
√CM244

F1=Toggle all

Selected WP Histories

AM242 AM242M AM243 C14 CA41..

The arrow keys are used to move up and down through the list. The user marks (i.e., selects) or unmarks radionuclides by pressing <ENTER> when the cursor is on that radionuclide. The <F1> key is used to mark or unmark all radionuclides. Hitting <ESC> exits the list with the new entries.

Define Realization Classes: This provides access to an input window for defining importance sampling of disruptive events. Importance sampling is discussed in detail in Appendix C of the RIP Theory and Capabilities Manual. Importance sampling of events allows the user to emphasize realizations in which relatively low probability events occur.

This increases the efficiency of the Monte Carlo sampling technique and improves the accuracy of the low probability tails of results distributions.

The user implements the event importance sampling technique by dividing all possible realizations into a number of *realization classes*, each realization class having a specified *pruning factor*. Realization classes are defined in terms of disruptive events. For example, suppose that the user has defined two types of disruptive events, referred to here as HUMAN and VOLCAN (specification of disruptive event types is discussed in Section 5.3). The user might then define one realization class to be "all realizations in which event VOLCAN occurs". By default, one class always exists which is called "all other realizations". In this case, this would include realizations in which either no disruptive events occurred or event HUMAN occurred.

Each disruptive event class is assigned a pruning factor (which must be greater than or equal to one). The pruning factor determines what fraction of the realizations in a given class are actually simulated. For example, if a class was assigned a pruning factor of 100, only one in every 100 realizations would actually be simulated, and the rest would be ignored. For a pruning factor of 1, every realization is simulated. To understand how this will affect the efficiency of the Monte Carlo sampling, refer again to the example above. Suppose that event VOLCAN was relatively rare (e.g., with a rate of occurrence of 10^{-7} per year). This would mean that for a 10,000 year simulation, there is only a 10^{-3} probability of realizing such an event. Hence, in order to properly represent this event in a Monte Carlo simulation, more than 10^3 realizations would have to be simulated. If, however, we were to specify a pruning factor of 1 for the class which consists of realizations with event VOLCAN, and a pruning factor of 100 for all other realizations, we would increase the frequency at which realizations in which VOLCAN occurred were simulated (by a factor of 100). In effect, if we had actually simulated 10^4 random realizations, it would seem that with respect VOLCAN type events we had simulated 10^6 random realizations. On the other hand, with respect to HUMAN realizations and all realizations in which no event had occurred, it would seem as if we had simulated somewhat less than 10^4 realizations (since we have artificially increased the rate at which we sampled VOLCAN realizations).

The user should consult Appendix C of the RIP Theory and Capabilities Manual for a more complete description of the event importance sampling algorithm.

Realization classes are defined in the following window:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Near Field Conditions	Waste Package Description	Make WP File		
WASTE PACKAGE MODEL				
REALIZATION CLASSES				
Events in Class				Class 1 of 2
volcan				
Pruning Factor : 1				
F1=Prev F2=Next F3=Add F4=Del F5=Display Events				

By default, a single realization class is originally defined, and this realization class is called "all other realizations". Additional classes can be added using the <F3> key. Defined classes can be browsed or deleted using the <F1>, <F2>, and <F3> keys. Note that regardless of how many classes are defined, the last class is always "all other realizations", and this name can not be changed. The pruning factor for this default class, however, can be edited. By default, the pruning factor for the first class is 1.

After defining a new class, the user must specify which events the class contains. This is done by typing in the name of the event (or events). Multiple events must be separated by commas (e.g., "VOLCAN, HUMAN"). *Only events that have been previously specified within the disruptive events input window (see Section 5.3) can be specified.* As a reminder, the <F5> key provides a list of all defined events for the user.

Make Waste Package Transfer File: Selecting this field creates a waste package transfer file. If any disruptive events have been defined under [Events], these will also be simulated, but any input pertaining to transport pathways and dose/risk are ignored. That is, the output is only in terms of release from the waste package.

Prior to creating the file, RIP goes through a series of data checks to ensure a consistent set of input. If any input errors are detected, creation of the file will be halted and an appropriate error message will appear alerting the user to the input error. If no input errors are detected, creation of the transfer file will commence. The progress of the transfer file creation is tracked on the screen by indicating which realization is currently being written.

When a transfer file is created, the RIP input file (.rp) is automatically saved and write-protected. This helps to ensure that the input file is consistent with the output file (which is created by the RIP back end based on the transfer file). This is necessary because both files are required in order to post-process results (as will be discussed in detail in Chapter 7). If the .rp file has been previously write-protected (i.e., a transfer file has been created with it previously), and the user attempts to create a transfer file again, the user is warned and must specifically indicate that he wants to override the write-protection.

The transfer file that is created is called NAME.BTF, where NAME is the name of the last input file specified by the user.

5.2 Input for the Radionuclide Transport Pathways Component Model

The transport algorithm implemented in RIP propagates mass along a network of interconnected *pathways*. The pathways reflect major features of the hydrologic system and are conduits through which mass transport occurs. As described in the Theory and Capabilities Manual, there are two types of transport pathways: *geosphere pathways* and *biocell pathways*.

Geosphere and biocell pathways are alternate models used by RIP to represent transport within and between environmental media. Most media can be represented using either type of pathway, but generally, geosphere pathways are used to represent subsurface hydrologic processes (such as fluid flow through an aquifer, or gaseous flow through rock), while biocell pathways are used to model transport between above-surface features (such as ponds, streams, and the atmosphere).

In a RIP application, the user defines a pathway network consistent with what is known about the geosphere and biosphere system. The pathways may be used both for flow balance and radionuclide transport purposes. They may account for either gas or liquid phase transport through the far-field.

RIP geosphere pathways can be further divided into interacting *flow modes*, which address heterogeneity at the local scale within a pathway (e.g., matrix flow and fracture flow might be two defined flow modes). The flow modes are primarily distinguished from one another based on flow velocity.

Concentration of radionuclides is tracked within all pathways. Knowing the radionuclide concentration, risk to potential receptor groups from any pathway (transport pathway or biosphere cell) can be assessed using the associated (optional) dose conversion table for the pathway. Dose conversion tables provide a linkage between concentration in a given pathway (e.g. groundwater) and potential receptors (e.g. children) considering the likely level of exposure (e.g. amount of radionuclide ingested per annum) to the receptor and the health risk from that level of exposure. Dose conversion tables are discussed in Section 5.4 of this manual, and in Chapter 6 of the RIP Theory and Capability Manual.

After carefully reading Chapter 4 of the RIP Theory and Capability Manual and achieving a clear understanding of the manner in which transport pathways are simulated in RIP, the user should next develop the conceptual model for the system which is to be represented, such that the various pathways and flow modes (and their associated parameters) are clearly defined. Only after developing and documenting a conceptual model for the pathway network should the pathway data be entered.

Selecting [Pathways] from the menu under [PA Model] provides access to the following input window:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Pathway Database Editor				
ID : SATUR1	Path 1 of 2		F1=Prev F2=Next F3=Add F4=Del F5=Path/ Cell F6=Goto F7=Insert F8=Copy	
DESC: flow in the saturated zone to stream				
Pathway Length (m): 15	(Constant)			
Total Area of Pathway (m ²): 200	(Constant)			
Total Volumetric Flow (m ³ *m/yr): Q1	(5)			
Define Discharge Pathways (STREAM,1.00)				
Define Flow Modes model				
Define Pathway Tolerance Values				
Dose Conversion Table (optional) :				
Output Selection				
Total Discharges : No	Discharges by RN : No			
Total Discharge Histories : No	Discharge Histories by RNs : No			

The user can add pathways with the <F3> key. Pathways can be deleted with the <F4> key. The <F1> and <F2> keys can be used to move between defined pathways.

The <F5> key is used to define a pathway as either a *geosphere pathway* or a *biocell pathway*. The window shown above is for the default choice (geosphere pathway). The biocell pathway window is shown below.

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Biosphere Cell Editor				
ID : STREAM	Path 2 of 2		F1=Prev F2=Next F3=Add F4=Del F5=Path/ Cell F6=GOTO F7=Insert F8=Copy	
DESC: stream downgradient from repository				
Annual Turnover Fraction (1/yr): 0.5	(Constant)			
Mass or vol. for concentrations : 1	(Constant)			
Mass of Sorbent (kg): 3	(Constant)			
Equilibrium Partition Coefficients				
Define Discharge Pathways (AE,1.00)				
Dose Conversion Table (optional) : table1				
Output Selection				
Total Discharge : No	Discharge by RN : No			
Total Discharge Histories : No	Discharge Histories by RNs : No			

The <F6> key allows the user to skip directly to a specified pathway. The <F7> key inserts a new pathway into the database before the pathway currently being viewed (otherwise, it is added to the end of the list). The <F8> key creates a new pathway (at the end of the list) which is identical to the pathway currently being viewed. The specific input fields for geosphere and biocell pathways are discussed in the following sections.

5.2.1 Geosphere Pathway Definition

The following input are required for geosphere pathways:

ID: This is a six character identifier for the pathway.

DESC: This is a 60 character description for the pathway.

Pathway Length: This is the actual length of the pathway (in m). The pathway length can be specified as a constant, a stochastic, a table, or a function. However, it must be specified as greater than zero. Note that this parameter may often be described directly as a time variable function (or it could be affected by disruptive events, as will be discussed in Section 5.3) such that the pathway length would actually change with time. (For example, a water table rise would have the effect of decreasing the length of an unsaturated zone pathway.) Shortening pathways in the middle of a simulation should be done very carefully, since this has the effect of immediately dumping a fraction of the mass in the pathway (equal to $\text{oldlength} - \text{newlength} / \text{oldlength}$) to the downstream pathway. Under some circumstances, this may result in artificially high releases. The manner in which RIP simulates such a change is detailed in Chapter 4 of the RIP Theory and Capabilities Manual.

As discussed in Section 6.2.1 of the RIP Theory and Capabilities Manual, the length of a pathway affects the manner in which concentrations (and hence doses) are computed, and should be specified carefully. In particular, *the pathway length should be such that the transit time through the pathway for the fastest radionuclide is no less than one timestep*. As discussed in that section, however, biocells can be appended to the end of pathways in order to modify the manner in which concentrations are computed.

Total Area of Pathway: This is the cross-sectional area of the pathway normal to the flow direction (in m^2). It can be specified as a constant, a stochastic, or a function. However, it must be specified as greater than zero.

Total Volumetric Flow: This is the total volumetric flow rate through the pathway (in m^3/yr). It can be specified as a constant, a stochastic, a table, or a function. However, it must be specified as greater than zero. Note, that as discussed in Section 4.4.2 of the RIP Theory and Capabilities Manual, RIP does not explicitly compute a water balance for the pathway network (although it does explicitly balance radionuclide mass). Hence, it is up to the user to define the water balance, if desired, through the specification of the pathway volumetric flow rates. These rates should be specified by the user such that they are interdependent and consistent (i.e., the flow in a particular pathway should be a function of the flows in the paths which discharge into it). The echo file created from within the [GENERAL] input window contains a concise summary of the specified flow balance.

Define Discharge Pathways: This provides access to a window for defining the pathways to which the current pathway discharges. It is discussed in more detail below in Section 5.2.1.1. Note that the specified discharge pathways (and their fractions) are listed directly below this field.

Define Flow Modes: This provides access to a window for specifying the characteristics of the pathway flow modes. It is discussed in more detail below in Section 5.2.1.2. Note that the specified flow modes are listed directly below this field.

Define Pathway Tolerance Values: This provides access to a window for specifying pathway tolerance values, which can increase the efficiency of the computational algorithm. This window is discussed in more detail below in Section 5.2.1.3.

Dose Conversion Table (Optional): If applicable, the name of the dose conversion table linking the pathway to receptor dose is entered here. Dose conversion tables are discussed in more detail in Section 5.4.2.

5.2.1.1 Pathway Network Definition

The pathway network is defined by identifying for each pathway one or more discharge pathways to which the mass is released.

Define Discharge Pathways: This provides access to the following window for specifying the pathways to which mass from this particular pathway is distributed upon discharge:

r [■] ————— Repository Integration Program (Rev. 4.04) —————

From pathway		SATUR1		Output Selection			
Discharge Pathway	Discharge Rule 1 of 1			Statistics		History	
	Fraction		Remaining	SUM	RNS	SUM	RNS
STREAM	0.4	(Constant)	1	Yes	Yes	No	No
AE	1	(Constant)	0.6	No	No	Yes	Yes
N/A		()					
		()					
		()					

Species following this rule : All
 AC227 AM241 AM242 AM242M AM243 C14 CA41 CL36 CM243 CM244 CM245 CM246 CO60
 CS135 CS137 H3 I129 MO93 NR-S1 NB93 NB94 NI-S1 NI59 NI63 NP236 NP237 PA231
 PB210 PD107 PU238 PU239 PU240 PU241 PU242 RA226 RA228 SE-S1 SE79 SM1...more

F1=Prev F2=Next F3=Add F4=Delete F5=Copy

Discharge pathways are specified in terms of *discharge rules*. A discharge rule is a set of discharge pathways that is applicable to a particular set of radionuclides. A discharge rule, however, can only be partitioned to pathways which have been previously defined. Hence, the user must define the pathways within the main [Pathways] input window before specifying the release rules here. The user can add and delete rules using the <F3> and <F4> keys, respectively. The <F1> and <F2> keys are used to move forward and backward among the defined rules.

The window will display all of the defined discharge pathways for the current rule, with the last entry being "N/A". To add an additional discharge pathway, place the cursor on "N/A". This is an option field, with the options being all of the available pathways (and the AE). After specifying the pathway ID, the user enters the fraction of the remaining balance which is allocated to this pathway. The remaining balance is indicated immediately to the right of the field.

For the last discharge pathway defined, the value automatically takes on the value of 1. For other pathways, however, this field can be specified as a parameter (a constant, a

stochastic, a table, or a function), with the constraint that it must *always* be greater than or equal to 0 and less than or equal to 1. Note that a total of nine discharge pathways can be specified for a given rule.

Entering the *fraction of remaining balance* (as opposed to the *actual fraction*) may appear somewhat awkward. However, this convention allows the fractions to be represented stochastically, while still ensuring that they total to one. This convention is used in several other places within the RIP user interface and its application is discussed further in Appendix B.

Note that geosphere pathways can discharge mass to other geosphere pathways, biocell pathways, or both.

As mentioned above, RIP automatically defines a special discharge location called AE, to which mass may discharge. This refers to the "accessible environment". The accessible environment can be assigned any meaning desired by the user, but is typically used to represent a regulatory boundary (e.g., the ground surface; some specified distance from the site).

For each defined rule, the user specifies whether All, Some or None of the radionuclides follow the rule. If only one rule has been defined, this is forced to All. When a new rule is added, the default value is None. To add radionuclides to a rule, move the cursor to this field and hit <ENTER>. This brings up a drop-down menu listing all radionuclides. The user marks (i.e., selects) or unmarks radionuclides by hitting <ENTER> when the cursor is on that radionuclide. The arrow keys are used to move up and down through the list. The <F1> key can be used to mark or unmark all radionuclides. Hitting <ESC> exits the list with the new entries.

The only way to delete a radionuclide from a rule is to add it to another rule (i.e., whenever a radionuclide is added to a rule, it is automatically deleted from the other rule). Note that in order to delete a rule, the user must first reassign all of the radionuclides associated with that rule (rules can only be deleted if they have no radionuclides associated with them).

The <F5> key copies all of the rules from another waste package or pathway. The user is prompted for the ID of the waste package or pathway from which the rules are to be copied. Note that all of the existing rules are replaced when the new rules are copied.

The right side of the window is used for output selection and is discussed below in Section 5.2.3.

5.2.1.2 Flow Mode Definition

For each geosphere pathway, it is necessary to specify one or more flow modes. As discussed in Chapter 4 of the RIP Theory and Capabilities Manual, the flow modes represent small-scale heterogeneities in the pathways.

Define Flow Modes: This provides access to the following window for specifying the characteristics of the pathway flow modes:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
Waste Package	Pathways	Events	Dose/Risk Make Transfer File
Pathway Database Editor			
ID : SATUR1	Path 1 of 2		F1=Prev F2=Next F3=Add F4=Del F5=Path/ Cell F6=Goto
DESC: flow in the saturated zone to stream			
Pathway Length (m): 15	(Constant)		
Total Area of Pathway (m ²): 200	(Constant)		
Total Volumetric Flow (m ³ m/yr): Q1	(5)		
Define Discharge Pathways (STREAM,1.00)			
Flow Modes			
Mode 1 of 1		F1=Prev F2=Next F3=Add F4=Del	
DESC: model			
Fraction of Total Flow remaining : 1			
Fraction of remaining Flow (0<x<1): 1	(Constant)		
Dispersivity (m): 0	(Constant)		
Poisson Transition Rate (1/m): MRATE	(0.001)		
Choose data type to input : Velocity			
Enter data value : MVEL	(0.0001)		
Define Retardation Factors			

The user can add flow modes with the <F3> key. Flow modes can be deleted with the <F4> key. The <F1> and <F2> keys can be used to move between defined flow modes.

The specific input fields associated with a particular flow mode are discussed below.

Description: This is a 60 character description for the flow mode.

Fraction of Remaining Flow: For each flow mode, the user specifies the fraction of the remaining balance which is to be allocated to this particular flow mode. The remaining balance is indicated in a display field directly above.

For the last flow mode defined, the value automatically takes on the value of 1. For other modes, however, this field can be specified as a parameter (a constant, a stochastic, a table, or a function), with the constraint that it must *always* be between greater than or equal to 0 and less than or equal to 1.

Entering the *fraction of remaining balance* (as opposed to the *actual fraction*) may appear somewhat awkward. However, this convention allows the fractions to be represented stochastically, while still ensuring that they total to one. This convention is used in several other places within the RIP user interface and its application is discussed further in Appendix B.

Dispersivity: This is the dispersivity (in m) for the one-dimensional advection-dispersion equation that is used to compute the breakthrough curve for the pathway. Note, however, that this field is relevant only when a single flow mode is defined for the pathway. If more than one flow mode is defined, this field is ignored and the breakthrough curve is calculated based on a Markov process algorithm. If only one mode is defined, however, and the dispersivity is non-zero, the

breakthrough curve is computed based on a one-dimensional solution for a tracer slug in an infinite domain with uniform flow. The one-dimensional advection-dispersion equation is described in Section 4.3.1.1 of the RIP Theory and Capability Manual. If a single flow mode is defined and the dispersivity is zero, the Markov process algorithm is used (in this case it would result in a plug-flow representation). The dispersivity can be specified as a constant, a stochastic, a table, or a function. However, it must be specified as non-negative.

Poisson Transition Rate: This is the Poisson transition rate described in Section 4.3.1.2 of the RIP Theory and Capability Manual. The transition rate has units of inverse length (m^{-1}). In basic terms, it represents the inverse of the length that we would expect a particle to travel in a particular flow mode before it transitions into a different flow mode within the pathway. The transition rate must be defined for one and only one flow mode within a pathway. (Whenever a flow mode's transition rate is specified, all other flow modes' rates are automatically set to zero in the user interface). The other transition rates are computed internally based on the one specified transition rate and the fraction of flow in each mode. The assumptions on which this calculation is based is detailed in Appendix G of the RIP Theory and Capabilities Manual. The transition rate which is defined by the user can be a constant, a stochastic, or a function. Note that if more than one flow mode is specified, the transition rate which is defined must be greater than zero.

Choose data type to input: For each flow mode, the user can choose to input either a velocity or an effective porosity to describe flow in the mode. The user uses the <PgUp> or <PgDn> keys to toggle between these two choices. The velocity and porosity are related as follows:

$$v_i = \frac{f_{Qi} Q}{An_i} \quad (5.9)$$

where:

- v_i = the average linear fluid velocity for flow mode i [m/yr];
- f_{Qi} = the fraction of the pathway volumetric flow in flow mode i;
- Q = the total pathway volumetric flow [m^3 /yr];
- A = the total pathway area normal to the flow direction [m^2]; and
- n_i = the effective porosity in flow mode i.

Enter data value: This is either the average linear flow velocity (in m/yr) or the effective porosity (unitless) for the flow mode, depending on the specification in the previous field. The value can be a constant, a stochastic, or a function. If specified as a velocity, it must be greater than zero. If specified as a porosity, it must be greater than zero and less than or equal to one.

Note that the user must be careful not to specify values for v_i , f_{Qi} , Q , and A such that n_i is greater than 1 (as this is physically unreasonable).

Define Retardation Factors: This provides access to the following window for specifying retardation factors:

Repository Integration Program (Rev. 4.04)			
General	FA Model	Strategy Model	Results
User's Guide Tutorial			
☐ Waste Package ☐ Pathways ☐ Events ☐ Dose/Risk ☐ Make Transfer File			
☐ Pathway Database Editor			
ID : SATUR1	Path 1 of 2		F1=Prev
DESC: flow in the saturated zone to stream			F2=Next
Pathway Length (m): 15	(Constant)		F3=Add
Total Area	☐ Retardation Factors		F4=Del
Total Volu	Group 1 of 1		F5=Path/
Define Dis	Sorption : 10	(Constant)	Cell
(STREAM,1	Matrix Diffusion : 20	(Constant)	F6=Goto
		F1=Prev F2=Next	
		Mode 1 of 1	
DESC: model			F1=Prev
Fraction of Total Flow remaining : 1			F2=Next
Fraction of remaining Flow (0<x<1): 1		(Constant)	F3=Add
Dispersivity (m): 0		(Constant)	F4=Del
Poisson Transition Rate (1/m): MRATE		(0.001)	
Choose data type to input : Velocity			
Enter data value : MVEL		(0.0001)	
Define Retardation Factors			

As discussed in Section 5.1.2.5, every element in the inventory of the specified waste packages is assigned to a *chemical element group*. Each chemical element group is referenced by an integer. Currently, RIP allows the user to specify up to 40 chemical element groups. In this window the user specifies retardation factors for each chemical element group. Note that, as a result, the retardation factors for any chemical element group can vary as a function of pathway and flow mode.

Two retardation factors must be specified: **Sorption** describes retardation due to chemical or physical sorption processes. **Matrix Diffusion** describes retardation due to matrix diffusion. The two retardation factors are combined as described in Appendix I of the RIP Theory and Capability Manual. Note that, in some cases, these two processes could potentially be represented by a single retardation factor. Both can be specified as constants, stochastics, tables, or functions. They must, however, be greater than or equal to one. Note that a retardation factor of 1 implies no retardation.

5.2.1.3 Definition of Pathway Tolerance Values

The last field in the pathway database editor window allows the user to specify pathway tolerance values:

Define Pathway Tolerance Values: This field provides access to the following window for specifying pathway tolerance values:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
Waste Package	Pathways	Events	Dose/Risk
Make Transfer File			
Pathway Database Editor			
ID : SATUR1	Path 1 of 2		F1=Prev
DESC: flow in the saturated zone to stream			F2=Next
Pathway Length	[]=PATHWAY TOLERANCE VALUES		F3=Add
Total Area of Pa	Pathway Length : 0.1	)	F4=Del
Total Volumetric	Flow Mode Velocity : 0.1	)	F5=Path/
Define Discharge	Flow Mode Porosity : 0.1		Cell
(STREAM,1.00)	Fraction of Total Flow : 0.1		F6=Goto
Define Flow Mode	Transition Rate : 0.1		F7=Insert
model			F8=Copy
Define Pathway Tolerance Values			
Dose Conversion Table (optional) : table1			
Output Selection			
Total Discharges : No	Discharges by RN : No		
Total Discharge Histories : No	Discharge Histories by RNs : No		

The use of tolerance values is discussed in Section 4.4.1.4 of the RIP Theory and Capabilities Manual. Tolerance values are a mechanism to increase the efficiency of the computational algorithm. Because transient changes in the pathway parameter values cause additional calculations to be performed in the RIP model (recalculation of the breakthrough curve), minimum (threshold) changes are required before the change is actually implemented in the simulation. The minimum required change is defined by the user in terms of the fractional difference between a new value and an old value. This fractional difference is computed as follows:

$$\Delta p = \frac{|p^{\text{new}} - p^{\text{old}}|}{\text{MIN}(p^{\text{new}}, p^{\text{old}})} \quad (5.10)$$

where:

Δp = the fractional difference for parameter p ;

p^{new} = the new value for parameter p ; and

p^{old} = the old value for parameter p .

The fractional difference, Δp , is compared to the user specified tolerance value to determine if the change should be implemented in the solution. If Δp does not exceed the tolerance value, p^{old} is not updated to p^{new} (the change is ignored).

As can be seen in the previous window, there are five tolerance values which must be specified. These must be specified as non-negative constants. Specification of 0 tolerance values ensures that all changes are implemented. The user should carefully define these values, considering the importance of different changes in the parameters if computational efficiency is of concern.

Tolerance values need only be specified for one pathway and are automatically copied and applied to the remaining pathways. The default values are 0.

Note that the breakthrough curves are always recalculated if the dispersivity (for single flow mode pathways) or retardation parameters are modified (the tolerance value for changes to the dispersivity or retardation factor is always zero and can not be changed by the user).

5.2.2 Biocell Pathway Definition

The following input are required for biocell pathways:

ID: This is a six character identifier for the pathway.

DESC: This is a 60 character description for the pathway.

Annual Turnover Fraction: Transport out of biocell pathways is modeled in a more simplified fashion than in geosphere pathways. Rather than specifying a series of transport parameters, the user specifies the fraction of radionuclides transported out of the cell each year. The value must be non-negative. A value of zero implies no radionuclides ever leave the cell. A value greater than one implies a turnover time of less than one year.

Mass or Vol. for Concentrations: RIP tracks the transport of *radionuclide mass* from one pathway to the next. In order to calculate a *concentration* of a radionuclide in a biocell pathway, RIP requires the user to input the *mass* or *volume* of the pathway. Depending on how the biocell has been defined by the user, concentrations could be computed either in mass per volume (e.g., for a stream), or mass per mass (e.g., for surface soils or biota). Note that the mass or volume specified here determines the concentration units for the pathway, which must be consistent with the units used in the dose conversion table (discussed below). The value must be non-negative.

Mass of Sorbent (kg): For biocells in which the concentration units are mass per volume of water (e.g., a lake, pond or stream), not all of the mass in the pathway will necessarily be dissolved. Some of the mass may be sorbed onto solids (sorbents) within the pathway (sediments within a pond).

Hence, this represents the mass of sorbent in the biocell pathway which can act to "buffer" the concentration in the water within the pathway (see Section 6.2.1 of the RIP theory and Capabilities Manual). It should be specified in units of kg. It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative.

Equilibrium Partition Coefficients (m^3/kg): This accounts for the fact that not all of the radionuclide mass in a fluid-filled biocell pathway will necessarily be dissolved. Some of it may be sorbed onto solids within the pathway. It should be specified in units of m^3/kg and pertains to the sorbent within the pathway. It can be described as a constant, a stochastic, or a function. It should always be specified as non-negative. As discussed in Section 6.2.1 of the Theory and Capabilities Manual, this term is nuclide specific.

Pressing this field provides access to the following window for specifying equilibrium partition coefficients:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
☐ Waste Package ☒ Pathways ☐ Events ☐ Dose/Risk ☐ Make Transfer File			
☐ Biosphere Cell Editor			
ID : STREAM	Path 2 of 2		F1=Prev
DESC: stream downgradient from repository			F2=Next
Annual Turnover Fraction (1/yr): 0.5	(Constant)		F3=Add
Mass o	Equilibrium Partition Coefficients		F4=Del
Mass o	Group 1 of 1		F5=Path/
Equili	Partition Coefficient (m3/kg) : KD1	(0.1)	Cell
Define	F1=Prev F2=Next		F6=GOTO
(AE,1.00)			F7=Insert
Dose Conversion Table (optional) :			F8=Copy
Output Selection			
Total Discharge : No	Discharge by RN : No		
Total Discharge Histories : No	Discharge Histories by RNs : No		

As discussed in Section 5.1.2.5, every element in the inventory of the specified waste packages is assigned to a *chemical element group*. Each chemical element group is referenced by an integer. Currently, RIP allows the user to specify up to 40 chemical element groups. In this window the user specifies equilibrium partition coefficients for each chemical element group.

Define Discharge Pathways: This provides access to a window for defining the pathways to which the current pathway discharges. It was discussed in detail in Section 5.2.1.1. Note that a biocell pathway can discharge to other biocell pathways, geosphere pathways, or both.

Dose Conversion Table (Optional): If applicable, the name of the dose conversion table linking the pathway to receptor health risk is entered here. Dose conversion tables are discussed in more detail in Section 5.4.2.

5.2.3 Saving Pathway Release Output

RIP allows two categories of pathway release outputs to be saved:

- releases *from* each pathway; and
- releases *from* each pathway *to* another pathway (or the AE).

Release from individual pathways is saved using the Output Selection fields at the bottom of the Pathways Database Editor (or Biosphere Cell Editor) menu, reproduced below:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
[]			
Waste Package	Pathways	Events	Dose/Risk
Make Transfer File			
[] Pathway Database Editor			
ID : SATUR1	Path 1	of 2	F1=Prev
DESC: flow in the saturated zone to stream			F2=Next
Pathway Length (m): 15	(Constant)		F3=Add
Total Area of Pathway (m ²): 200	(Constant)		F4=Del
Total Volumetric Flow (m ³ m/yr): Q1	(5)		F5=Path/
Define Discharge Pathways (STREAM,1.00)			Cell
Define Flow Modes			F6=Goto
model			F7=Insert
Define Pathway Tolerance Values			F8=Copy
Dose Conversion Table (optional) :			
Output Selection			
Total Discharges : Yes	Discharges by RN	: Yes	
Total Discharge Histories : No	Discharge Histories by RNs	: No	

Four options are available:

- Selecting Yes for "Total Discharges" saves the cumulative release for the current pathway summed over all radionuclides.
- Selecting Yes for "Total Discharge Histories" saves the time history of release for the current pathway summed over all radionuclides.
- Selecting Yes for "Discharges by RN" saves the cumulative release for the current pathway by radionuclide.
- Selecting Yes for "Discharge Histories by RN" saves the time history of release for the current pathway by radionuclide.

As discussed in Section 5.5, the radionuclides for which results are saved are selected in the Main Output Selection window.

Releases from a particular pathway to another pathway can be saved from within the Define Discharge Pathways Window, shown below:

r[■] Repository Integration Program (Rev. 4.04)

From pathway SATUR1				Output Selection			
Discharge Pathway	Discharge Rule 1 of 1			Statistics		History	
	Fraction		Remaining	SUM	RNS	SUM	RNS
STREAM	0.6	(Constant)	1	Yes	Yes	No	No
AE	1	(Constant)	0.6	No	No	Yes	Yes
N/A	(	)					
	(	)					
	(	)					

Species following this rule : All
 AC227 AM241 AM242 AM242M AM243 C14 CA41 CL36 CM243 CM244 CM245 CM246 CO60
 CS135 CS137 H3 I129 MO93 NB-S1 NB93 NB94 NI-S1 NI59 NI63 NP236 NP237 PA231
 PB210 PD107 PU238 PU239 PU240 PU241 PU242 RA226 RA228 SE-S1 SE79 SM1...more

F1=Prev F2=Next F3=Add F4=Delete F5=Copy

There are four options:

- Selecting Yes under "Statistics" and "Sum" saves the cumulative release *from* the current pathway *to* the specified discharge pathway summed over all radionuclides.
- Selecting Yes under "History" and "Sum" and "saves the time history of release *from* the current pathway *to* the specified discharge pathway summed over all radionuclides.
- Selecting Yes under "Statistics" and "RNs" saves the cumulative release *from* the current pathway *to* the specified discharge pathway by radionuclide.
- Selecting Yes under "History" and "RNs" saves the time history of release *from* the current pathway *to* the specified discharge pathway by radionuclide.

As discussed in Section 5.5, the radionuclides for which results are saved are selected in the Main Output Selection window.

5.3 Input for the Disruptive Events Component Model

Selecting [Events] from the menu under [PA Model] provides access to input windows for describing the disruptive events component model.

Prior to entering data into RIP, the user must first have a good understanding of the manner in which RIP simulates the occurrence and consequences of disruptive events. Chapter 5 of the RIP Theory and Capabilities Manual describes the theory and discusses the assumptions on which the RIP disruptive events algorithms are based,

Disruptive events are defined here as discrete perturbations of the repository system. That is, disruptive events are discrete occurrences which have some quantifiable effect on the processes described by the other two component models. Note that discrete is a relative term, and does not necessarily imply instantaneous (e.g., given the long time scales of interest, something

taking place over a period of 100 years could be considered as a discrete event). Examples of disruptive events under this definition include volcanism, faulting, and human intrusion. In general, however, the disruptive events component model is intended to represent relatively rare occurrences. Events that occur continuously throughout the time period of interest are more efficiently modeled as processes within the other two component models.

The occurrence of disruptive events is described as follows:

- The user defines all significant events (i.e., all events which are both credible and consequential).
- Each significant event must be assigned a *rate of occurrence*. Event occurrences are simulated as Poisson processes.
- Each disruptive event can be assigned one or more *descriptor parameters*. Descriptor parameters define the characteristics and/or the magnitude of the event. For example, the list of descriptor parameters for a volcanic event might include dike length and dike width.

For each disruptive event, there are four types of internally-defined disruptive event *consequences* which describe *discrete responses*:

- The radionuclides in a number of waste packages are moved directly to the accessible environment.
- The radionuclides in a number of waste packages are moved directly to a specified pathway (e.g., the saturated zone).
- A number of waste packages are disrupted in place.
- A portion of the mass (previously released from waste packages) contained within a pathway is immediately discharged to another pathway (which may represent the accessible environment).

In addition to the four discrete response consequences described above, it is also possible to directly influence parameters defined in the waste package and transport pathways components, and this capability can be used to specify *long-term consequences* (e.g., a permanent water table rise).

Selecting [Events] from the main menu provides access to the following input window:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Disruptive Event Window				
Parameter ID : VOLCAN (must be "Event" type)			Event 1 of 1	
Description : volcanism				
Annual Rate of Occurrence : RATE2			(1.0E-7)	
Can Event Reoccur : Yes				
Define Event Descriptors				
DIKEL				
Event Consequences				
Move WPs to AE				
Move WPs to a pathway				
Disrupt WPs				
Move Contents of pathway to another pathway				
Modify Parameters				
			F1=Prev F2=Next F3=Add F4=Del	

The user can add disruptive events with the <F3> key. Events can be deleted with the <F4> key. The <F1> and <F2> keys can be used to move between defined events.

The specific input fields in the disruptive event window shown above are discussed in the following sections.

5.3.1 Event Definition

Parameter ID: This is the name of the disruptive event parameter. This must correspond to an event type parameter in the parameter module database. (Recall that the user can enter the parameter module to define such a parameter by hitting <Alt>-<P>.) As described in Section 4.3.4, definition of an event parameter requires a short description, a rate of occurrence, and specification of whether the event can reoccur.

Note that the fields in the disruptive events window directly below "Parameter ID" ("Description", "Annual Rate of Occurrence", and "Can Event Reoccur") can not be edited here. They are displayed based on the information specified when the event parameter was defined within the parameters module.

During a simulation, when an event parameter is used in a function (i.e., when it affects some other parameter), the value of the event parameter is a function of time, taking on one of two values: it is equal to one if the event has occurred during the current timestep; and it is equal to zero if it has not occurred during the current timestep.

Note that an event with a rate of occurrence less than 10^{-10} is ignored by the disruptive events module (even if pruning factors are used). Note also that RIP only recognizes one event per timestep. That is, if the rate of occurrence is such that more than one event occurs per timestep, only a single event is actually simulated.

5.3.2 Definition of Event Descriptors

Define Event Descriptors: This field provides access to the following window for defining event descriptors:

Repository Integration Program (Rev. 4.04)	
General	PA Model Strategy Model Results
User's Guide Tutorial	
☐ Waste Package ☐ Pathways ☒ Events ☐ Dose/Risk ☐ Make Transfer File	
☒ Disruptive Event Window	
Parameter ID : VOLCAN	(must be "Event" type) Event 1 of 1
Description : volcanism	
☒ Event Descriptors	
Parameter ID : DIKEL	(1000) Descriptor 1 of 1
Description : dike length (m)	
F1=Prev F2=Next F3=Add F4=Del	
DIKEL Event Consequences Move WPs to AE Move WPs to a pathway Disrupt WPs Move Contents of pathway to another pathway Modify Parameters	
F1=Prev F2=Next F3=Add F4=Del	

The user can add descriptor parameters with the <F3> key. Descriptor parameters can be deleted with the <F4> key. The <F1> and <F2> keys can be used to move between defined descriptors. Note that the specified descriptors are listed directly below the *Define Event Descriptors* access field.

Only stochastic parameters can be defined as descriptor parameters. The user must define these parameters using the parameters module. As discussed in Chapter 5 of the RIP Theory and Capability Manual, descriptor parameters allow the user to define the characteristics and/or the magnitude of a disruptive event. It is intended that descriptor parameters be used to help define the magnitude of the consequences. The magnitude of a consequence can then be described as a function of the characteristics of that particular event. For example, for a volcanic intrusion event, we might want to describe the number of waste packages which are disrupted as a function of the geometry and size of the dike. Descriptor parameters would then be defined which describe the dike size and geometry.

Descriptor parameters are realized every time the particular event occurs. Note, however, that sampling biasing (described in Section 4.3.3.1) is never applied to descriptor parameters.

Descriptor parameters should only be used to define event consequences. That is, they should not be referenced elsewhere within the model (in cases where they are, the initial value is used for the entire realization).

5.3.3 Definition of Event Consequences

As shown in the main disruptive event window, five types of event consequences can be defined. These each have a separate input window. The first four describe discrete event occurrences. The last window allows the user to directly modify other system parameters.

Note that only descriptor parameters are realized every time a particular event occurs within a realization. If the user wants consequences to be realized every event occurrence, the consequences (or the parameters describing them) must be specified as descriptor parameters.

If the event has not occurred, all consequences are automatically set to zero. The default value for all consequences is zero.

Move WPs to AE: This provides access to the following input window:

Repository Integration Program (Rev. 4.04)	
General	PA Model Strategy Model Results
User's Guide Tutorial	
Waste Package	Pathways Events Dose/Risk Make Transfer File
Disruptive Event Window	
Parameter ID : VOLCAN	(must be "Event" type) Event 1 of 1
Description : volcanism	
Annual Rat	Move WPs to AE
Can Event	Number of WPs moved : WPMOVE (0.5)
Define Event Descriptors	
DIKEL	
Event Consequences	
Move WPs to AE	
Move WPs to a pathway	
Disrupt WPs	
Move Contents of pathway to another pathway	
Modify Parameters	
F1=Prev F2=Next F3=Add F4=Del	

This moves a specified number of waste packages directly to the accessible environment. The waste packages which are moved are chosen randomly from each specified waste package group. It is assumed that the inventory released from each package which is moved is equal to the inventory of an *unfailed* package at the time of the event. Note that the total number of waste packages remaining in the repository is not updated (reduced) subsequent to an event (it is assumed that the number of waste packages which are moved is a small fraction of the total).

The user can specify the number of waste packages as a constant, a stochastic, or a function (e.g., of descriptor parameters). It cannot, however, be described as a function of an event type parameter. Furthermore, the value must be greater than or equal to 0.

Move WPs to a pathway: This provides access to the following input window:

Repository Integration Program (Rev. 4.04)	
General	PA Model Strategy Model Results
User's Guide Tutorial	
[■] Waste Package Pathways Events Dose/Risk Make Transfer File	
[■] Disruptive Event Window	
Parameter ID : VOLCAN (must be "Event" type) Event 1 of 1	
Description : volcanism	
Annual Rat	[■] Move WPs to a Pathway
Can Event	Pathway Name : SATUR1 Path 1 of 2
	Number of WPs moved : 2 (Constant)
Define Event	
DIKEL	
Event Consequences	
Move WPs to AE	
Move WPs to a pathway	
Disrupt WPs	
Move Contents of pathway to another pathway	
Modify Parameters	
F1=Prev F2=Next F3=Add F4=Del	

This moves a specified number of waste packages directly to a specified pathway. The waste packages which are moved are chosen randomly from each specified waste package group. It is assumed that the inventory released from each package which is moved is equal to the inventory of an *unfailed* package at the time of the event. It is also assumed that all of the waste package's inventory is immediately released to the pathway (i.e., the waste package is completely disrupted during the movement and release of the contents is not limited by any alteration, dissolution, or mass transfer processes at the waste package). Note that the total number of waste packages remaining in the repository is not updated (reduced) subsequent to an event (it is assumed that the number of waste packages which are moved is a small fraction of the total).

When running RIP without the pathways component, this consequence is not incorporated into the simulation.

Waste packages can be moved to any of the pathways which have been previously defined by the user. The user can browse through the pathways using the <F1> and <F2> keys.

The user can specify the number of waste packages as a constant, a stochastic, or a function (e.g., of descriptor parameters). It cannot, however, be described as a function of an event type parameter. Furthermore, the value must be greater than or equal to 0.

Disrupt WPs: This provides access to the following input window:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
☐ Waste Package ☐ Pathways ☐ Events ☐ Dose/Risk ☐ Make Transfer File			
☐ Disruptive Event Window			
Parameter ID : VOLCAN (must be "Event" type)		Event 1 of 1	
Description : volcanism			
Annual R	☐ Disrupt WPs		
Can Even	Number of WPs disrupted : DISRUP (4)		
Define Event Descriptors			
DIKEL			
Event Consequences			
Move WPs to AE			
Move WPs to a pathway			
<u>Disrupt WPs</u>			
Move Contents of pathway to another pathway			
Modify Parameters			
			F1=Prev F2=Next F3=Add F4=Del

This instantaneously disrupts a specified number of waste packages in place. The waste packages which are disrupted are chosen randomly from each specified waste package group. Only an integer number of waste packages can be disrupted (non-integer numbers are truncated). It is assumed that both the primary and secondary container are disrupted.

NOTE: Due to computational considerations, RIP currently only fails the secondary container within primary containers which were not failed prior to the disruptive event. For example, if all of the primary containers had failed prior to the event (due to corrosion processes), but the secondary containers (i.e., cladding) were assumed to still be intact, this consequence would have no effect on the secondary containers. If, however, the primary containers had not failed previously, the event would instantaneously fail the specified number of both the primary and secondary containers. This approximation only becomes important if the secondary container has a long lifetime after the primary container has failed. In this situation, it may be more appropriate to treat such a consequence conservatively by actually moving the waste packages to the first discharge pathway.

The user can specify the number of waste packages as a constant, a stochastic, or a function (e.g., of descriptor parameters). It cannot, however, be described as a function of an event type parameter. Furthermore, the value must be greater than or equal to 0.

Move Contents of pathway to another pathway: This provides access to the following input window:

Repository Integration Program (Rev. 4.04)	
General	PA Model Strategy Model Results
User's Guide Tutorial	
Waste Package	Pathways Events Dose/Risk Make Transfer File
Disruptive Event Window	
Parameter ID : VOLCAN	(must be "Event" type) Event 1 of 1
Description : volcanism	
Annual Rate	= Move contents of One Pathway to Another Pathway
Can Event	1 of 1
Define Event	Disrupted Pathway Name : SATUR1
DIKEL	Receiving Pathway : AE (or AE)
Event Consequences	Frac of balance moved : 0.01 (Constant)
F1=Prev. F2=Next F3=Add F4=Delete	
Move WPs to AE Move WPs to a pathway Disrupt WPs Move Contents of pathway to another pathway Modify Parameters	
F1=Prev F2=Next F3=Add F4=Del	

This moves a specified fraction of the total mass in a specified pathway directly to another pathway (which may represent the accessible environment). Mass can be moved from/to any of the pathways which have been previously defined by the user. The user can browse through the pathways using the <F1> and <F2> keys.

The user can specify a constant, a stochastic, a table, or a function (e.g., of descriptor parameters). It cannot, however, be described as a function of an event type parameter. Furthermore, the value must be greater than or equal to 0 and less than or equal to one.

Note that the fraction of the mass which is moved pertains to the remaining balance. For example, if two events occur in a single timestep, each of which moves 0.6 of the mass from a particular pathway (which, say, totals 100 units), this would be interpreted as follows: first move $0.6(100) = 60$ units of mass would be moved; then 0.6 of the remaining balance (40 units) would be moved (24 units), leaving 16 units of mass in the pathway.

Modify Parameters: This provides access to the following input window:

Repository Integration Program (Rev. 4.04)	
General	PA Model Strategy Model Results
User's Guide Tutorial	
Waste Package	Pathways Events Dose/Risk Make Transfer File
Disruptive Event Window	
Parameter ID : VOLCAN	(must be "Event" type) Event 1 of 1
Description : volcanism	
Annual Rate	= Parameters modified by Event
Can Event	Parameter ID : WLELVL Parameter 1 of 2
Define Event	Sensitivity : Add
DIKEL	Value : DELH (20)
F1=Prev F2=Next F3=Add F4=Del F5=Insert	
Event Consequences	
Move WPs to AE Move WPs to a pathway Disrupt WPs Move Contents of pathway to another pathway Modify Parameters	
F1=Prev F2=Next F3=Add F4=Del	

This window allows a user to modify a system parameter contained in the parameters module database by specifying its sensitivity to the occurrence of the disruptive event. The user does this by modifying the specified sensitive parameter using an *influence parameter* (shown as "Value" in the screen above). The sensitivity can take one of three forms: whenever the disruptive event occurs, the user-defined influence parameter can *replace*, *multiply*, or be *added* to the original parameter value.

The user can modify as many parameters as desired. The user can add sensitive parameters (to the end of the list) with the <F3> key. The <F5> key can be used to insert a sensitive parameter into a particular position in the list. Sensitive parameters can be deleted with the <F4> key. The <F1> and <F2> keys can be used to move between defined sensitive parameters.

For each sensitive parameter, the following information is required:

Parameter ID: This is the name of the sensitive parameter. Note that this must be a previously defined parameter within the parameter database. Furthermore, it can not be a function or event type parameter. Only stochastic and constant parameters can be modified (a function type parameter must be modified by modifying its independent variables). Note also that any parameter specified as a descriptor parameter cannot be modified.

Sensitivity: This is an option field which the user toggles (using the <PgUp> or <PgDn> keys) to choose the manner in which the influence parameter modifies the sensitive parameter (Add, Multiply, or Replace).

Value: This is the influence parameter. It can be specified as a constant or a parameter. If specified as a parameter, it can be a constant, a stochastic, or a function. It cannot, however, be specified as a function of an event type parameter. For any given event occurrence, parameters are modified *after* the four instantaneous consequences are evaluated. Hence, if a consequence is a function of a modified parameter, the new value of the modified parameter will not be used until the next event occurrence. Likewise, parameters are modified in the order that they are listed. Hence, if *Value* (the influence parameter) for the first modified parameter is a function of the second modified parameter, the new value of the second modified parameter will not be used by the first until the next event occurrence.

It is worth noting how *Modify Parameters* can be used to keep a running total of the number of events which have occurred during the current realization. The user defines a parameter (e.g., TOTVOL) and specifies it as a constant equal to 0. He/she then specifies that this parameter is modified as follows:

Repository Integration Program (Rev. 4.04)	
General	PA Model Strategy Model Results
User's Guide Tutorial	
Waste Package	Pathways Events Dose/Risk Make Transfer File
Disruptive Event Window	
Parameter ID : VOLCAN (must be "Event" type) Event 1 of 1	
Description : volcanism	
Annual Rate	Parameters modified by Event
Can Event	Parameter ID : TOTVOL Parameter 2 of 2
Define Event	Sensitivity : Add
Value : 1 (Constant)	
DIKEL	F1=Prev F2=Next F3=Add F4=Del F5=Insert
Event Consequences	
Move WPs to AE	
Move WPs to a pathway	
Disrupt WPs	
Move Contents of pathway to another pathway	
Modify Parameters	
F1=Prev F2=Next F3=Add F4=Del	

Note that the influence parameter is equal to one, which is added to TOTVOL every time the event occurs. TOTVOL will then be the running total of the number of occurrences of event VOLCAN for each realization. The user may then wish use describe other parameters as a function of TOTVOL (e.g., a particular process may be a function of how many times the event has occurred to date). Also, as will be discussed in Section 7, the final value of TOTVOL for each realization can be viewed when processing results.

5.4 Input for the Dose/Risk Component Model

Selection of [Dose/Risk] from the menu under [PA Model] accesses input windows used to describe the dose or health risk to individuals resulting from exposure to concentrations of radionuclides within geosphere and/or biocell pathways. Input for this component model is divided into two categories: [Receptors], and [Dose Conversion Tables]. Each of these categories is discussed in detail below. Modeling the dose and/or health risk with RIP is discussed in detail in Chapter 6 of the RIP Theory and Capabilities Manual.

5.4.1 Receptors Database

5.4.1.1 Defining Receptors

The first step in defining a dose/risk model is to define the *receptor groups* who may potentially be exposed to the doses. Selecting [Receptors] accesses the following input window:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
Select Output				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
Receptors Database				
Receptor ID : KIDS			Receptor 1 of 2	
Description :				
Risk/Dose Ratio : 1			(Constant)	
Number of individuals in receptor group : 0				
F1=Previous Receptor F2=Next Receptor F3=Add Receptor F4=Delete Receptor				
Output Selections				
Peak dose/risk statistics : Yes		Peak dose/risk statistics by RN : Yes		
Total dose/risk histories : Yes		Dose/risk histories by RN : Yes		
Mean total risk history : Yes		Mean dose/risk hist by RN : Yes		

The user can add receptors with the <F3> key. Receptors can be deleted with the <F4> key. The <F1> and <F2> keys can be used to move between defined receptors.

The input fields in the receptor database editor window shown above are discussed below:

Receptor ID: This is a six character identifier for the receptor.

Description: This is a 60 character description for the receptor.

Risk/Dose Ratio: Also referred to as a *risk factor*, this converts the annual effective dose equivalent for a particular receptor group (e.g., in Sv/yr) to the annual incremental cancer risk for a member of the group (see Section 6.3 of the RIP Theory and Capabilities Manual). The units of the risk factor are inverse dose (e.g., Sv^{-1} or mrem^{-1}). The risk factor can be a constant, a stochastic, a table, or a function. It must be a positive value. Note that if the user wishes to generate results in terms of dose (rather than risk), a risk factor of 1 should be specified (although the post-processor will still label results as risk).

Number of individuals in receptor group: This field is used in calculating Total Population Risk. For each receptor group, the total number of individuals can be specified, and the total risk summed over the population. The calculation of total population risk is discussed in greater detail in Section 5.5.

5.4.1.2 Saving Receptor Output

Depending on how dose conversion factors are specified (see Section 5.4.2), the user can choose to compute either concentrations, doses or risks associated with a particular receptor. The output which is saved is specified using the fields in the Output Selection sub-window. Six options are available:

- Selecting Yes for "Peak Dose/Risk Statistics" saves the peak concentration/dose/risk for the current receptor summed over all radionuclides.
- Selecting Yes for "Total Dose/Risk Histories" saves the time history of concentration/dose/risk for the current receptor summed over all radionuclides.

- Selecting Yes for "Mean Total Risk" saves the time history of concentration/dose/risk for the current receptor summed over all radionuclides, and averaged over all realizations. To compute the average, RIP saves the time history data for all realizations and calculates the average value at each time step.
- Selecting Yes for "Peak Dose/Risk Statistics by RN" saves the peak concentration/dose/risk for the current receptor by radionuclide.
- Selecting Yes for "Dose/Risk Histories by RN" saves the time history of concentration/dose/risk for the current receptor by radionuclide.
- Selecting Yes for "Mean Dose/Risk History by RN" saves the time history of concentration/dose/risk for the current receptor summed over all radionuclides, and averaged over all realizations. To compute the average, RIP saves the time history data for all realizations and calculates the average value at each time step.

As discussed in Section 5.5, the radionuclides for which results are saved are selected in the Main Output Selection window.

5.4.2 Dose Conversion Tables

Dose conversion tables provide the link between concentration of a radionuclide in the environment and the dose received by a potential receptor. That is, a dose conversion factor converts a concentration in some environmental media (represented by a geosphere or biocell pathway) to a dose received by a member of a receptor group.

For example, if a local lake has some concentration of ^{241}Am , a member of a receptor group could receive a dose of ^{241}Am from the lake in several ways, including ingestion, drinking the water, eating fish from the lake, and immersion by swimming in the water.

The dose received by a receptor is a function of the receptor group. For example, children typically spend more time swimming than adults, so the dose they receive from a given concentration of radionuclide in the lake might be higher than an adult. Similarly, fishermen tend to spend more time around water and would also likely receive a correspondingly higher dose.

Dose is a function of radionuclide type. Less active radionuclides give smaller doses of radioactivity. Also, some radionuclides are not as readily absorbed by species in the food chain. For example, if ^{241}Am and ^{14}C were present in at the same concentration in a lake, they would not necessarily be present at the same concentration in the flesh of a fish taken from that lake.

Dose is a function of the nature of the biocell or geosphere pathway. For example, the same concentration of a radionuclide in a deep aquifer, not used as a source of drinking water, would result in a different dose conversion than an aquifer used as drinking water source. Also, similar concentrations of radionuclides in a lake and in topsoil may result in very different levels of dose to receptors.

In RIP, dose conversion tables are organized by pathway. Each geosphere or biocell pathway can be assigned one conversion table. Where appropriate, several pathways can share a single dose conversion table. The name of the dose conversion table for a pathway is designated when defining the pathway (see Section 5.2.1 and 5.2.2 for more details).

Selecting [Dose Conversion Tables] accesses the following input window:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
[] Waste Package Pathways Events <u>Dose/Risk</u> Make Transfer File			
[] Receptors <u>Dose Conversion Table</u>			
Table: TABLE1		Table 1 of 1	
Desc.: F1=Prev table F2=Next table F3=New table F4=Delete table			
Receptor	Dose/Concentration ratio		
	Species: AC227 (1 of 55)		
KIDS	1.5	(Constant)	
ADULTS	0.5	(Constant)	
	0	(Constant)	
	0	(Constant)	
	0	(Constant)	F7=Copy ratio to all Species
	0	(Constant)	F8=Load ratio from RN extra data
	0	(Constant)	(requires non-N/A value to work)
	0	(Constant)	F9=Set N/A (no doses) for this
	0	(Constant)	receptor in this table
	0	(Constant)	
	F5=Prev species F6=Next species		

The user can add tables by pressing the <F3> key. Tables can be deleted by pressing <F4>. The <F1> and <F2> keys can be used to move between defined tables. The input fields in the dose conversion table window shown above are discussed below:

ID: This is a six character identifier for the dose conversion table.

DESC: This is a 60 character description of the dose conversion table.

For each table, dose conversion numbers are entered for each receptor for each radionuclide. Each column of a dose conversion table represents a different radionuclide while each row represents a different receptor. The window allows editing of one column of the table at a time. <F5> and <F6> keys are used to toggle between various radionuclides (columns) within a single table. The <F7> key allows the user to copy the ratios defined for the current radionuclide to all species.

The units for dose conversion factors are defined by the user in terms of annual effective dose equivalent divided by concentration (e.g., [Sv/yr]/[g/m³]). For a geosphere pathway, the concentration units are always g/m³, and the dose conversion factor must be defined accordingly. For a biocell pathway, the user defines the concentration units directly (when specifying the mass or volume for the pathway, as discussed in Section 5.2.2), and the dose conversion factor must be consistent with these units.

In the dose conversion table window, the cursor must be placed on a specific row of the table (there is one row for each receptor). The <F8> key provides a mechanism for importing data from the species table:

```
[■] _____ Repository Integration Program (Rev. 4.00 )
      General          PA Model          Strategy Model       Results
                        Version 4.00 Features

[■] _____
Waste Package    Pathways    Events    Dose/Risk    Make Transfer File

[■] _____
Receptors                Dose Conversion Table
[■] _____ Dose/Concentration Conversion Table _____
Table: water                                Table 1   of 1
Desc.: Dose Conversion for water ingestion [(mrem/yr)/(g/m**3)]
===== F1=Prev table F2=Next table F3=New table F4>Delete table =====
Receptor- Dose/Concentration ratio -----
Species: AC227 (1 of 55 )
ADULT N/A (N/A )
      0 (Constant )
      0 (Constant )
      0 (Constant )
      0 (Constant )
      0 (Constant ) F7=Copy ratio to all Species
      0 (Constant ) F8=Load ratio from RN extra data
      0 (Constant ) (requires non-N/A value to work)
      0 (Constant ) F9=Set N/A (no doses) for this
      0 (Constant ) receptor in this table
      0 (Constant )
F5=Prev species F6=Next species
```

Pressing <F8> will bring up a dialog box, which lists the headings for all of the “extra” user-defined columns in the species table:

```

[■] Repository Integration Program (Rev. 4.00 )
      General          PA Model          Strategy Model          Results
                          Version 4.00 Features

[■] Waste Package      Pathways      Events      Dose/Risk      Make Transfer File

[■] Receptors          Dose Conversion Table

[■] Dose/Concentration Conversion Table

Table: water                      Table 1      of 1
De

Rec: Enter number of the pathway dose-conversion factor to use
      to autoloa all factors for receptor ADULT
      0 : specific-activity values (Ci/g)
      AD 1 : DCF#1 2 : DCF#2
      Selection:

      0          (Constant )      F9=Set N/A (no doses) for this
      0          (Constant )      receptor in this table
      0          (Constant )

F5=Prev species F6=Next species
rk)

```

By selecting one of these options, the dose conversion factors from the species table are copied into the interface for that receptor. NOTE: All of the entries are automatically multiplied by the

specific activity when copied from the species table. Hence, the units for the values in the species table should be (dose/yr)/(Ci/volume or mass), where the "volume or mass" has the same units as the pathway where the dose is calculated (e.g., m³ for a geosphere pathway; kg for a soil biocell). When using the <F8> key, a special option is always available (0) that copies the specific activities to the dose conversion table. This causes the results to be expressed in units of concentration (in Ci/volume or mass).

The <F9> key allows the user to remove an entire row (i.e., all the values pertaining to a particular receptor) from a dose conversion table. This is done when a particular dose conversion table only applies to certain receptors. Although this same thing could be accomplished by simply specifying zero values for that row, using the <F9> key causes the program to skip the calculations completely, thereby increasing computational efficiency.

5.5 Making a Total System Transfer File

Selecting [Make Transfer File] from the main menu provides access to the input windows for specifying general information regarding the creation of total system transfer file. Having done so, the user can then create the transfer file from this window.

The input window is as follows:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
PERFORMANCE MODEL				
Number of timesteps : 100				
Length of timestep (yrs) : 100				
Number of realizations : 1000				
Run using expected values : No				
Allow RN decay in pathways : Yes				
WP Release				
Select Desired Output				
Define Realization Classes				
Create Transfer .BTF file				

Number of timesteps: This is the number of timesteps to be simulated. It must be greater than or equal to one. The beginning of the simulation (time = 0) is defined as the time of closure.

Length of timestep: This is the timestep length in years. It must be non-negative.

Number of realizations: This is the number of Monte Carlo realizations to be simulated. It must be greater than or equal to one.

Run using expected values: This is an option field which is answered Yes or No. If Yes, a single realization using the expected value for all stochastic parameters is produced (and the previous input specifying the number of realizations is ignored). Note that this

realization is generally close to the median realization, which is generally lower than the mean realization (since the mean is strongly affected by extreme realizations).

Allow RN Decay in Pathways: This is an option field which turns on or off (the default is on) radioactive decay while radionuclides are within the transport pathways. Note that decay within the waste package prior to reaching the pathways is unaffected.

WP Release: This provides access to the following window:

☐ Repository Integration Program (Rev. 4.04)	
☐ General	☐ PA Model
☐ Strategy Model	
☐ User's Guide Tutorial	
☐ Waste Package	☐ Pathways
☐ Events	☐ Dose/Risk
☐ Make Transfer File	
☐ PERFORMANCE MODEL	
Number of timesteps	: 100
Length of timestep (yrs)	: 100
Number of pathways	: 1000
Number of values	: No
Number of pathways	: Yes
☐ WP Release	
Run WP Model?	: Yes
Containment Time (yr)	: 100
Release Type	: Fractional
Release Value (1/yr)	: 0.00001
☐ Create Transfer .BTF file	

This window provides the user with an option to skip simulation of the waste package behavior and radionuclide release model. It requires the following input:

Run WP Model? If this option field is answered Yes, the transfer file that will be created will be a total system transfer file (both the waste package and the pathways will be simulated). The remaining fields in this window are then ignored. If this option field is answered No, waste package failure and mass exposure and release are not explicitly simulated. The mass is still released to the pathways specified by the user. However, a user-specified waste package release rate is assumed. The form of this user-specified constant release rate is defined by the following fields.

Containment Time: This is the containment time in years. No mass is released until this time is reached. Once this time is reached, however, mass is released from the waste packages at the constant release rate specified below. This must be specified as a non-negative constant.

Release Type: Two types of user-specified waste package release rates are allowed. The type of release, specified by this option field, is either "Fractional" or "Constant". If "Fractional" is specified, the constant release rate for each radionuclide per waste package is equal to a user-specified RELEASE VALUE multiplied by the inventory (in grams) in an unfailed waste package *at the containment time specified above*. If "Constant" is specified, the constant release rate for each radionuclide per waste package is equal to the user-specified RELEASE VALUE, and is completely independent of the specified inventories.

Release Value: This is the user-specified RELEASE VALUE discussed above. If Fractional is specified, it has units of 1/yr. If Constant is specified, it has units of g of each RN/yr.

Note that the total repository release rate for each radionuclide is equal to the constant release rate described above multiplied by the total number of packages in the repository. Also note that when using the option to bypass the waste package model, the total inventory cannot be exhausted (it is assumed to be unlimited, although for "fractional" releases, the release rate is dependent on the specified inventory).

Select Desired Output: This provides access to an input window for defining the form of the output:

SELECT DESIRED OUTPUTS					
Waste Pkg. Rel. rate 10 CFR 60.113 : Yes	Cum. release to Acc. Env. 40 CFR 191 : Yes		Normalize by Table 1 Yes		
Standard Outputs		Statistics		Time History	
		Sum	by RN	Sum	by RN
Total Release from all Waste Packages		Yes	Yes	Yes	Yes
Total Release to the AE		Yes	Yes	Yes	Yes
Release from each Waste Package		On	On	AsIs	On
Release from each Pathway		On	On	AsIs	On
Conc/Dose/Risk for each Receptor		On	On	AsIs	On
Selected Pathways		Selected Pathway Histories			
Selected Waste Packages		Selected WP histories			
Selected Receptors		Selected Receptor Histories			
		Selected Parameter Histories			
Select Species : All AC227 AM241 AM242 AM242M AM243 C14 CA41..					
Total Population Risk : No					

The user chooses the exact outputs that are to be saved in the results file. Note that choosing all of the available outputs could create very large output files.

The top portion of the window is used to select regulatory output.

Cum. release to A.E. (40 CFR 191.13): This saves the cumulative release to the accessible environment (normalized to the 40 CFR 191.13 limit). Normalization of results is discussed in detail in Appendix C. For each realization, a single value for the cumulative radionuclide release (i.e., summed over all timesteps and all radionuclides) is saved.

Waste Pkg. Rel. rate (10 CFR 60.113): This saves the maximum annual radionuclide release rate (normalized to the 10 CFR 60.113 limit) achieved by any radionuclide over the length of the realization. Normalization of results is discussed in detail in Appendix C. For each realization, the single maximum annual release value and the ID of the radionuclide having the maximum annual release are saved. In addition, RIP also saves three other values for each realization: the time at which the

maximum release occurred, the fraction of primary containers which have failed by 300 years, and the fraction of primary containers which have failed by 1000 years (these latter two can be used to evaluate "substantially complete containment").

Normalize by Table 1: This determines whether or not the cumulative radionuclide release results described below are to be normalized. It does not pertain to the "Waste Package Release Rate" described above. If the user selects Yes, the cumulative releases below are normalized to the 40 CFR 191.13 limit (normalization is discussed in detail in Appendix C). If the user selects No, results are output in units of Curies.

Time histories are not applicable to the 10 CFR 60.113 output. To save a time history for the 40 CFR 191.13 output, the user should select "Sum" "Time History" for "Total Release to the AE". When results are normalized, this output is identical to the 40 CFR 191.13 output.

Two types of "Standard Outputs" are available: Statistics and Time History data. The results under "Cumulative Releases" in the "Statistics" column refer to results that are summed over all timesteps. That is, they are cumulative with respect to time. "Sum" indicates that results are summed over all radionuclides, while "by RN" indicates that a separate cumulative release is to be saved for each specified radionuclide. Results under the "Time History" column are saved at each timestep. "Sum" indicates that results are summed over all radionuclides, while "by RN" indicates that a separate set of release data is to be saved for each specified radionuclide. If "by RN" is selected, only those radionuclides chosen in the "Select Species" window at the bottom of the screen will be saved.

For each category for which time history data is selected, time histories are saved only for those realizations that contain the five highest cumulative normalized releases (40 CFR 191.13).

Total Release From all Waste Packages: This saves the cumulative waste package release summed over all waste package groups, and can be saved at each time step and/or summed over the entire realization. If "Sum" is selected the cumulative waste package release (summed over all radionuclides) is saved for each realization. If "by RN" is selected the cumulative waste package release for each individual specified radionuclide is saved on each realization. Hitting <ENTER> on the field will bring up a pull-down menu with the choices "Yes" and "No". The arrow keys can be used to select the desired option.

Total Release to the AE: This saves the total cumulative release to the accessible environment, and can be saved at each time step and/or summed over the entire realization. If "Sum" is selected the cumulative release to the accessible environment (summed over all radionuclides) is saved for each realization. If "by RN" is selected the cumulative release to the AE for each individual specified radionuclide is saved on each realization. Hitting <ENTER> on the field will bring up a pull-down menu with the choices "Yes" and "No". The arrow keys can be used to select the desired

option. Note that if results are being normalized, "Sum" provides the same results as "Cum. release to A.E (40 CFR 191.13)" specified above.

Release from each Waste Package: This saves the cumulative waste package release for each waste package group, and can be saved at each time step and/or summed over the entire realization. If "Sum" is selected the cumulative waste package release (summed over all radionuclides) is saved for each group on each realization. If "by RN" is selected the cumulative waste package release for each individual specified radionuclide is saved for each group on each realization. This line serves as a global override for options specified in the individual Waste Package windows. Note that this does not include "From-To" type results (e.g., "from waste package A to pathway B"). Hitting <ENTER> on the field will bring up a pull-down menu with the choices "On", "Off", or "AsIs". The arrow keys can be used to select the desired option. "AsIs", which is the default, saves results only for those items specified in the individual Waste Package windows. If "On" is selected, all results are saved for the specified option, while if "Off" is selected, none of the results are saved for the specified option, regardless of the settings within the Waste Package window.

Release From each Pathway: This saves the cumulative release from each specific pathway, and can be saved at each time step and/or summed over the entire realization. If "Sum" is selected the cumulative release from each pathway (summed over all radionuclides) is saved for each realization. If "by RN" is selected the cumulative release from each pathway for each individual specified radionuclide is saved on each realization. This line serves as a global override for options specified in the individual Pathways windows. Note that this does not include "From-To" type results (e.g., "from pathway A to pathway B"). Hitting <ENTER> on the field will bring up a pull-down menu with the choices "On", "Off", or "AsIs". The arrow keys can be used to select the desired option. "AsIs", which is the default, saves results only for those items specified in the individual Pathways windows. If "On" is selected, all results are saved for the specified option, while if "Off" is selected, none of the results are saved for the specified option, regardless of the settings within the Pathways window.

Conc./Dose/Risk for each Receptor: This saves the *peak concentration/dose/risk* for each receptor, the mean risk histories (including standard deviation of risk) for all receptors, and the total risk histories for each receptor. Mean risk histories are based on the mean risk value (over all realizations) at each timestep. The value presented here may represent the risk, dose, or concentration to the given receptor, depending upon the values specified for the dose/concentration and risk/dose factors. For a more detailed discussion of the relationship between risk, dose and concentration, refer to Chapter 6 of the RIP Theory and Capabilities manual.

If "Sum" is selected the peak value (summed over all radionuclides) is saved for each realization. If "by RN" is selected the peak value for each individual specified radionuclide is saved on each realization. This line serves as a global override for options specified in the individual Receptors windows. Hitting <ENTER> on the

field will bring up a pull-down menu with the choices "On", "Off", or "AsIs". The arrow keys can be used to select the desired option. "AsIs", which is the default, saves results only for those items specified in the individual Receptor windows. If "On" is selected, all results are saved for the specified option, while if "Off" is selected, none of the results are saved for the specified option, regardless of the settings within the Receptor window.

If either of the "Time History" options are set to "Yes", both Mean Total Risk History and Total Risk History will be activated for all receptors.

The next section provides access to windows which summarize all of the output selection options which were specified in other windows. Selecting a field (e.g., "Selected Waste Packages") accesses a window which summarizes all of the output options selected in the other windows (e.g., the Waste Package and Define Discharge Pathways windows):

Repository Integration Program (Rev. 4.04)		
SELECT DESIRED OUTPUTS		
Waste Pkg. Rel. rate 10 CFR 60.113 : No	Cum. release to Acc. Env. 40 CFR 191 : No	Normalize by Table 1 No
Discharge from Waste Packages: Total discharge from SPENT Discharge by RN from SPENT to AE Total discharge from HLDW		
Selected Pathways Selected Waste Packages Selected Receptors		Selected Pathway Histories Selected WP histories Selected Receptor Histories Selected Parameter Histories
Select Species : All AC227 AM241 AM242 AM242M AM243 C14 CA41..		
Total Population Risk : No		

Select Species: The "Select Species" key is used to choose those radionuclides for which results are to be saved for all options which have been specified as "by RN". The two available options are All and Some. Placing the cursor to this field and hitting <ENTER> brings up a drop-down menu listing all radionuclides:

Repository Integration Program (Rev. 4.04)

SELECT DESIRED OUTPUTS

Waste Pkg. Rel. rate 10 CFR 60.113 : No	Cum. release to Acc. Env. 40 CFR 191 : No	Normalize by Table 1 No
--	--	----------------------------

Standard Outputs	Statistics		Time History	
	Sum	by RN	Sum	by RN
Total Release from all Waste Packages	Yes	No	Yes	No
Total Release to the AE	No	No	Yes	No
Release from each	AsIs	AsIs	AsIs	AsIs
Release from each	AsIs	AsIs	AsIs	AsIs
Conc/Dose/Risk fo	AsIs	AsIs	AsIs	AsIs

Selected Pathways	Selected Pathway Histories
Selected Waste Pa	Selected WP histories
Selected Receptor	Selected Receptor Histories
	Selected Parameter Histories

AM242	AM242M	AM243	C14	CA41
CL36	CM243	CM244		
CM244				

F1=Toggle all

The arrow keys are used to move up and down through the list. The user marks (i.e., selects) or unmarks radionuclides by pressing <ENTER> when the cursor is on that radionuclide. The <F1> key is used to mark or unmark all radionuclides. Hitting <ESC> exits the list with the new entries.

Total Population Risk: This field is used to calculate the total risk to a population, summed over the course of the entire simulation. The total population consists of the summation of the populations of each receptor. The formula used to calculate the unitless total population risk is as follows:

$$\text{Total Population Risk} = \sum_{i=1}^N [\text{POP}_i * R_i * (\sum_{t=1}^T \text{DOSE}_i(t) * \Delta t)] \quad (5.11)$$

where:

- POP_i = the population of receptor i;
- R_i = the Risk/Dose ratio for receptor i [e.g., Sv⁻¹];
- N = the total number of receptors;
- T = the total number of time steps;
- DOSE_i(t) = the dose to receptor i at time t [e.g., Sv/yr]; and
- Δt = the length of time step [yr].

Define Realization Classes: This provides access to an input window for defining importance sampling of disruptive events. Importance sampling is discussed in detail in Appendix C of the RIP Theory and Capabilities Manual. Importance sampling of events allows the user to emphasize realizations in which relatively low probability events occur.

This increases the efficiency of the Monte Carlo sampling technique and improves the accuracy of the low probability tails of results distributions.

The user implements the event importance sampling technique by dividing all possible realizations into a number of *realization classes*, each realization class having a specified *pruning factor*. Realization classes are defined in terms of disruptive events. For example, suppose that the user has defined two types of disruptive events, referred to here as HUMAN and VOLCAN (specification of disruptive event types is discussed in Section 5.3). The user might then define one realization class to be "all realizations in which event VOLCAN occurs". By default, one class always exists which is called "all other realizations". In this case, this would include realizations in which either no disruptive events occurred or event HUMAN occurred.

Each disruptive event class is assigned a pruning factor (which must be greater than or equal to one). The pruning factor determines what fraction of the realizations in a given class are actually simulated. For example, if a class was assigned a pruning factor of 100, only one in every 100 realizations would actually be simulated, and the rest would be ignored. For a pruning factor of 1, every realization is simulated. To understand how this will affect the efficiency of the Monte Carlo sampling, refer again to the example above. Suppose that event VOLCAN was relatively rare (e.g., with a rate of occurrence of 10^{-7} per year). This would mean that for a 10,000 year simulation, there is only a 10^{-3} probability of realizing such an event. Hence, in order to properly represent this event in a Monte Carlo simulation, more than 10^3 realizations would have to be simulated. If, however, we were to specify a pruning factor of 1 for the class which consists of realizations with event VOLCAN, and a pruning factor of 100 for all other realizations, we would increase the frequency at which realizations in which VOLCAN occurred were simulated (by a factor of 100). In effect, if we had actually simulated 10^4 random realizations, it would seem that with respect VOLCAN type events we had simulated 10^6 random realizations. On the other hand, with respect to HUMAN realizations and all realizations in which no event had occurred, it would seem as if we had simulated somewhat less than 10^4 realizations (since we have artificially increased the rate at which we sampled VOLCAN realizations).

The user should consult Appendix C of the RIP Theory and Capabilities Manual for a more complete description of the event importance sampling algorithm.

Realization classes are defined in the following window:

Repository Integration Program (Rev. 4.04)				
General	PA Model	Strategy Model	Results	
User's Guide Tutorial				
Waste Package	Pathways	Events	Dose/Risk	Make Transfer File
REALIZATION			PERFORMANCE MODEL	
			Number of timesteps	: 100
			Length of timestep (yrs)	: 100
CLASSES			Class 1 of 2	
Events in Class				
volcan				
Pruning Factor : 1				
F1=Prev F2=Next F3=Add F4=Del F5=Display Events				

By default, a single realization class is originally defined, and this realization class is called "all other realizations". Additional classes can be added using the <F3> key. Defined classes can be browsed or deleted using the <F1>, <F2>, and <F3> keys. Note that regardless of how many classes are defined, the last class is always "all other realizations", and this name can not be changed. The pruning factor for this default class, however, can be edited. By default, the pruning factor for the first class is 1.

After defining a new class, the user must specify which events the class contains. This is done by typing in the name of the event (or events). Multiple events must be separated by commas (e.g., "VOLCAN, HUMAN"). *Only events which have been previously specified within the disruptive events input window (see Section 5.3) can be specified.* As a reminder, the <F5> key provides a list of all defined events for the user.

Create Transfer File: Selecting this field creates a transfer file. Prior to creating the file, RIP goes through a series of data checks to ensure a consistent set of input. If any input errors are detected, creation of the file will be halted and an appropriate error message will appear alerting the user to the input error. If no input errors are detected, creation of the transfer file will commence. The progress of the transfer file creation is tracked on the screen by indicating which realization is currently being written.

When a transfer file is created, the RIP input file (.rp) is automatically saved and write-protected. This helps to ensure that the input file is consistent with the output file (which is created by the RIP back end based on the transfer file). This is necessary because both files are required in order to post-process results (as will be discussed in detail in Chapter 7). If the .rp file has been previously write-protected (i.e., a transfer file has been created with it previously), and the user attempts to create a transfer file again, the user is warned and must specifically indicate that he wants to override the write-protection.

The transfer file that is created is called NAME.BTF, where NAME is the name of the last input file specified by the user.

5.6 Creating a Transfer File From the Command Line

RIP provides the capability to generate transfer files directly from the DOS command line without having to manually open the front-end. This can be very useful, particularly when multiple runs are being executed (perhaps in a batch file being run overnight). This can be accomplished by typing the command:

```
RIP inputfile -t
```

where "input file" is the name of the .rp file. When this is done, the RIP front-end will automatically load and generate the transfer file. All of the prompts that are typically issued when creating a transfer file are skipped. However, if an input file error is detected, a message will be issued and the transfer file will not be generated. In this instance, the execution of a batch file would also be halted.

5.7 Running the Back End Program

After creating a transfer file, the back end program must be run to carry out the actual simulations and produce a results file (as discussed in Section 2.3). The back end can be run by typing the following command:

```
RIP2 -4 inputfile
```

where "inputfile" is the name of the *transfer file*. Note that the name of the executable RIP backend file is RIP2.EXE.

The executable file need not be present in the active directory when the command is typed, as long as the executable is in the path (typing "path" at the DOS prompt will show the current path). Note that, regardless of whether RIP is on the path, the user can type the full pathname for the executable (e.g., "c:\programs\rip\rip2 -4 inputfile"). Note, however, that the input files for the backend (the *.btf and *.bpf files) must be in the active directory.

A number of command line flags can also be set in order to modify the behavior of the back end programs.

A summary of all the command line flags can be seen by typing

```
RIP2 -?
```


usage: RIP2 [-2 file] [-4 file] [-ceEfgmPpqrstvz1?]

The following command line flags are recognized:

- 2 file Redirect stderr (standard error) to file.*
- 4 file RIP transfer file*
- c col This column gets all the mass.
- e Echo input to stderr, other results to stdout.*
- E Echo input to stdout -- don't do anything.*
- f Flush stdout after each realization.
- g Produce time history in grams.
- m Report available memory (Borland C only).
- P file Write risk data to file
- p num Write risk data for radionuclide # num
- q num Write risk data for receptor # num
- r Terminate lines with CR/LF.
- s Status report to display.*
- t generate ASCII transfer file*
- v Display program version*
- z Turn off decay.*
- 1 Run one realization only.
- ? Display this help message.*

Many of these flags are primarily programmer's tools and are not documented here. Those flags which the user will find useful are highlighted (with a *) above and summarized below:

RIP2 -2 err.out -4 test.btf

This command will read the transfer file "test.btf", send standard error messages to "err.out". Note that if the standard error messages are not redirected to files, by default they will be printed to the screen.

RIP2 -E -2 echo.out -4 test.btf

This command will read the transfer file "test.btf" and create an echo file (which is sent to "echo.out"). After writing the echo file, it will terminate (i.e., it will not actually carry out a simulation). Hence, this is merely a way to create an echo file to verify that the transfer file has been read properly. The content of the echo file is similar (although more terse) than that of the front end echo file created using the [GENERAL] input window.

RIP2 -e -2 err.out -4 test.btf

This command will read the transfer file "test.btf", and send standard error messages to "err.out". In addition, the input is echoed to the error message file "err.out".

RIP2 -s -4 test.btf

This is the most common command line for running the back end. This command will read the transfer file "test.btf", send standard error messages to "err.out". In addition, the progress of the simulation (realization number and timestep) is sent to the display screen. Note, however, that this option will tend to slow execution somewhat (on the order of 10%).

RIP2 -v

This command will display the version number of the program which you have.


```
RIP2 -z -2 err.out -4 test.btf
```

This command will read the transfer file "test.btf", and send standard error messages to "err.out". In addition, radioactive decay will be disabled. This command line flag (-z) has precedence over the front end option described in Section 5.5 ("Allow RN Decay in Pathways"). It pertains to both the waste package and the pathways.

```
RIP2 -t -4 test.btf
```

This command will read the transfer file "test.btf". In addition, it will create an ASCII version of the transfer file called "test.asc". An ASCII version of the transfer file can be used by experienced RIP users to debug a dataset.

5.8 Input Documentation

It is useful to summarize here the manner in which the input into RIP can be documented by the user. As has been discussed in previous sections, the front end provides three mechanisms for documentation:

- The user can create an echo file from within the [General] input window. This creates an ASCII file summarizing in readable format all of the input parameters specified by the user. This is the most complete and easiest method for documenting input files.
- The user can create summaries of the parameter database using the <F6> key from within the parameters module. This essentially results in a subset of the information contained in the echo file described above.
- The user can save to a file and/or print every input window using the <Ctrl>-<F> and <Ctrl>-<P> keys.
- The user can create an echo file using the "-E" or "-e" command line flag when running the back end (RIP2).

5.9 Combining Parameter Databases

In some cases, several users may want to input data for the same RIP application (e.g., one person working on pathways, another working on the waste package). Unfortunately, due to the interdependence of the various component models, it is not possible to combine the waste package input from one .rp file with the pathways or disruptive events input from another. It is possible, however, to combine the *parameter databases* of two .rp files, and this can be useful in many cases.

To use this capability, hit <F1> from the top level menu of RIP (i.e., the menu line which shows [General], [PA Model], [Strategy Model], and [Results]). You will be prompted for the .rp file to from which you wish to copy the parameter database. RIP will merge the parameter database

from the selected file with that of the current file. If there are duplicate parameter names in the two databases, the parameter from the file being copied will be ignored (the parameter in the current file will be unchanged).

After merging the files, be sure to use <Alt>-<S> to save the changes.

5.10 Using RIP with Non-Radioactive Species

RIP outputs cumulative release results in terms of Curies, since its primary purpose is to simulate repositories (or hazardous waste sites) containing radioactive species. It is also possible, however, to use RIP to model nonradioactive species (e.g., organic compounds at a hazardous waste site).

In order to model non-radioactive species with the current version of RIP, it is simply necessary to specify the specific activity as 1 and run the back-end using the -z command line flag (no decay). (Results, however, will still be labeled as Ci by the post processor).

Decay rates may still be used if appropriate (i.e., if the decay is first-order). In some cases, specification of daughter products may also be appropriate (e.g., one species being chemically or biologically transformed into another).

6. DATA ENTRY AND APPLICATION OF THE STRATEGY EVALUATION MODEL

Strategy modeling is a very powerful tool available as part of the RIP model. The user can use the RIP strategy module to evaluate the probable cost, time, and effect of a strategy. This chapter discusses the RIP strategy model and its use.

A strategy, as used in RIP, refers to a set of activities or elements that are to be carried out in order to develop a better understanding of the proposed repository system. The elements of a strategy represent activities such as the following:

- A test or set of tests that are intended to provide additional information about one or more of the parameters that define the performance model. Note that such tests do not always provide information regarding RIP parameters directly.
- Development of an improved model that will reduce overall model uncertainty. For example, an activity could consist of developing and making a number of runs of a lower-level model of a subsystem. The result might be a modified component model in RIP, or improved parameter precision, or reduced model-error.
- Construction of an infrastructure element (e.g. a borehole, or a road), or completion of a require

RIP's strategy module allows the user to define strategies, and to evaluate their effectiveness by examining probability distributions of four specific results:

- the cost of executing the strategy;
- the duration of the strategy;
- the strategy's likely effect on RIP model parameters; and
- the strategy's likely effect on the performance model's predictions.

Each of these four results is evaluated by RIP as a stochastic variable. Thus RIP provides the user with probability distributions for the overall cost and distribution of a strategy. Similarly, RIP provides the user with probability distributions of what the model parameter or model performance measure distributions may look like after the strategy is executed. The last item is complex; it represents our probabilistic estimate *now* of what our probabilistic performance estimate will be in the *future*.

The issue of uncertainty in the cost and duration of a strategy is important. While it is convenient to plan using fixed times and costs, reality is far less certain. The cost and time required to carry out any activity (drill a borehole, carry out a research program, obtain a regulatory permit) is not fixed and generally beyond the control of an agency developing a repository. The RIP strategy model contains what is, in effect, a version of the *Critical Path Method* that incorporates *uncertainty*.

6.1 Defining a Strategy

The user enters the strategy model by selecting [Strategy Model] from the top level menu. This brings up the *Strategy Activities Editing* menu shown below. The current element number and the total number of available elements are shown in the upper right portion of the editing window.

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
STRATEGY ACTIVITIES EDITING			
Element Id : A	Is element active: Yes	Element 1 of 2	
Element Desc: strategy element A			
Element Cost : COSTA	1000	F1=Prev F2=Next F3=Add F4=Delete F5=Copy Strategy 	
Element Time : TIMEA	10		
Planned Start: 0	(years)		
Precedent Elements 1: B			
Parameters Changed 1: FLOW			
F6=Calculate cost/time distributions		F7=display costs F8=display times	

An element can be added by pressing <F3>. It is not necessary to press <F3> to create the first element. RIP readies the first element for editing when the user enters the strategy module. An element can be deleted by pressing <F4>. The <F5> key can be used to copy a strategy from a different .rp file. <The <F6>, <F7>, and <F8> keys are used for computing and displaying cost and time (duration) distributions, and are discussed in more detail in Section 6.2.1.

The user can select an element for editing by pressing <F1> and <F2> to browse forward and backward until the element of interest is brought to the screen. Having brought the element of interest to the screen, there are several areas of the *strategy activities editing* window requiring input or editing. These are described below.

Element ID: This is the six character identifier for the element.

Element Desc: This is a 60 character description for the element.

Is element active: This is an option field which can be toggled Yes or No (using the <PgUp> or <PgDn> keys). This option allows the user the opportunity to store strategies that are not currently in use, rather than deleting them.

Element Cost: This is the estimated cost of the element (in any consistent unit). It can be described as a constant, a stochastic, a table, or a function. It should always be specified as non-negative. It can not be described as a direct function of time, but it may be described as a function of element duration, discussed below.

Element Time: This is the estimated duration of the element (in years). It can be described as a constant, a stochastic, a table, or a function. It should always be specified as non-negative.

Planned Start: This is the planned start time (typically in years from the present time). It can be described as a constant, a stochastic, a table, or a function.

Precedent Elements: If multiple elements have been defined, it is possible to define precedence relationships between them. For a given element, the user can define one or more precedent elements. For each precedent element, the user can require that the given element not be executed or completed until:

- the precedent element has completed execution;
- the precedent element has begun execution; or
- a specified number of years after the precedent element has begun or completed execution.

The precedent elements feature allows the user to create a precedence network similar in form to the Critical Path Method while incorporating path uncertainty.

The precedent element window is shown below:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
STRATEGY ACTIVITIES EDITING			
Element Id : A	Is element active: Yes	Element 1 of 2	
Element Desc: strategy element A			
Element Cost : COSTA	1000	F1=Prev F2=Next F3=Add F4=Delete F5=Copy	
Element Time : TIMEA	10		
Planned Start: 0	(years)		
Precedent Elements 1: B			
Parameters Changed 1: FLOW			
Precedent Element 1 of 1			
Element Id : B	Precedent element reference point : Finish	F1=Prev	F2=Next
	Current element reference point : Start	F3=Add	F4=Del
	Time Gap between reference points : 2	Constant	

Element ID: This is the ID for the precedent element. The user defines a precedent element by entering the ID of any previously defined element (in this case B).

Reference points and time gap: The reference points are option fields with two choices (Start or Finish). In the example shown, the precedent element's reference point is "Finish" while the current element's reference point is "Start". The time gap between reference points is 2. This means that element A (the current element) cannot be started until 2 years after the finish of the precedent element.

Alternatively, a precedent element reference point of "Start" and a time gap of 0 would imply that the current element starts at the same time as the precedent element. *Note that precedent requirements can push a Planned Start backward (larger values) but can not move it forward.*

The user can toggle between using Start or Finish as a reference point by moving to the appropriate field and pressing <Enter> and using the <Up> and <Down>

arrows to move within the list. Alternatively, the <PgUp> and <PgDn> keys can be used to toggle. The time gap between reference points can be entered in the usual manner as a constant, a function, a table, or a stochastic parameter.

Additional precedent elements can be defined by pressing <F3>. Elements can be deleted by pressing <F4>. The user can browse through (and edit) the existing precedent elements by pressing <F1> or <F2>.

Parameters Changed: This field provides access to a window for specifying how parameters would be changed by carrying out the element. The user can define parameters which may change as a result of strategy execution, and describe how they may change:

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
User's Guide Tutorial			
STRATEGY ACTIVITIES EDITING			
Element Id : A	Is element active: Yes	Element 1 of 2	
Element Desc: strategy element A			
Element Cost : COSTA	1000	F1=Prev F2=Next F3=Add F4=Delete F5=Copy Strategy F8=display times	
Element Time : TIMEA	10		
Planned Start: 0	(years)		
Precedent Elements 1: B			
Parameters Changed 1: FLOW			
Parameter Id: FLOW		Parameter 1 of 1	
Information change: 1		Constant	
F1=Prev	F2=Next	F3=Add	F4=Delete

Any *stochastic* parameter in the parameter database can be changed as a result of a strategy. Multiple parameters can be affected by a strategy. Additional parameters to be changed can be selected by pressing <F3>, as indicated at the bottom of the menu shown above. Parameters can be deleted by pressing <F4>. The user can browse (and edit) parameters to be changed by pressing <F1> or <F2>.

Parameter ID: This is the name of the parameter which is changed due to the strategy element.

Information change: This represents the change in knowledge gained from execution of a strategy element. Information change is the ratio of the *test standard deviation* to the current *parameter standard deviation*. Hence, an information change equal to one implies that the test provided an amount of information equal to that currently supplied; a information change of less than one implies that the test provided a larger amount of information than that currently supplied; and a information change of greater than one implies that the test provided a smaller amount of information than that currently supplied. An information change of 0 implies that the test was definitive (i.e., there would be no remaining uncertainty after the test).

A more detailed explanation of information change can be found in Chapter 7 of the RIP Theory and Capabilities Manual.

6.2 Evaluating the Effects of a Carrying out a Strategy

As described in Section 6.1, the RIP strategy model allows the user to evaluate the effectiveness of a strategy by examining probability distributions of four specific results:

- the cost of executing the strategy;
- the duration of the strategy;
- the strategy's likely effect of RIP model parameters; and
- the strategy's likely effect on the performance model's predictions.

This section describes how to execute a RIP strategy and view the results obtained.

6.2.1 Strategy Time and Cost

Strategy time and cost distributions are obtained directly from within the *strategy model window*. Once the strategy has been entered, the user can calculate strategy cost and duration by pressing <F6>, as indicated on the strategy model window shown in Section 6.1. Note that only elements that are marked "Active" are included. The user is prompted for the number of strategy realizations. The user also has the option of computing costs and times for all active elements or only those active elements up to an including the one currently shown in the window.

Once calculated, strategy cost is displayed by pressing <F7>, while strategy duration is displayed by pressing <F8>. RIP output for both cost and duration are presented as stochastic parameters. Displaying stochastic parameters is discussed in Section 4.4.

6.2.2 Effect of a Strategy on Individual Parameters

When in the parameters module (the user can enter the parameters module from most places in the RIP front end by pressing <Alt>-<P>), the user can view the effect of a strategy on a particular parameter by pressing <F9>. Pressing <F9> brings up the *Strategy Results Display* window shown below.

Repository Integration Program (Rev. 4.04)						
General		PA Model		Strategy Model		Results
Parameter Editing						
STRATEGY RESULTS DISPLAY						
Plot type	:	CDF	----- Plot Range -----		----- Data Range -----	
X-axis	:	Linear 0	100	1.005439	99.5523	
Y-Axis	:	Linear 0	1.	0	1	
Grid	:	Yes				
Title	:	Strategy for FLOW: 1000 realizations, 102 loops				
X-axis Title	:	Parameter FLOW: repository flow rate				
Prob = Original	Distribution Following Characterization Strategy					
value		0.01	0.10	0.50	0.90	0.99
0.001: 1.014246		1.018599	1.059687	1.145076	1.518899	14.04686
0.01 : 1.065663		1.38506	1.643181	1.986266	4.27664	26.39364
0.05 : 1.280933		1.732003	1.908239	2.019589	16.76098	44.67358
0.10 : 1.596989		1.888484	2.077087	2.404834	26.28536	51.76257
0.25 : 3.082288		2.664131	2.970639	4.382365	47.49398	66.49604
0.50 : 11.22756		5.682879	6.656012	9.933654	65.44502	77.56182
0.75 : 35.04466		13.64114	15.06624	22.25352	79.67664	89.05392
0.90 : 65.59133		23.75803	25.60819	39.93279	90.85036	95.75713
0.95 : 79.24156		29.29466	30.27238	49.09061	95.00809	97.88088
0.99 : 95.81898		47.0705	48.65886	67.55105	98.66696	99.28183
0.999: 99.36111		65.92487	77.61389	96.56393	99.78593	99.93514
F1=Screen Plot F2=HardCopy Plot						

The left-hand side of the strategy results display window shows the *original* CDF of the parameter (i.e. prior to execution of the strategy), while the right hand side shows the probability of the new distribution of the parameter following execution of the strategy. In particular, the right hand columns show the probability of a particular quantile level for the parameter after execution of the strategy (i.e., probabilities of probabilities). For example, in the screen shown above, the original distribution of the parameter was such that at the 0.99 probability level, the value was 95.8. The columns to the right indicate that after carrying out the strategy, there will be a 0.01 probability that the 0.99 probability level will be less than 47.07, a 0.10 probability that it will be less than 48.6, a 0.50 probability that it will be less than 67.5, a 0.90 probability that it will be less than 98.6, and a 0.99 probability that it will be less than 99.2.

A screen or hard copy plot of the information described above can be obtained by pressing either <F1> or <F2> respectively. Default plot scale axes and titles are selected but can be overridden by the user by moving to the appropriate field and entering a new value. Linear or logarithmic plot axes can be chosen by moving to the appropriate field and pressing either <PgUp> or <PgDn>. The user can obtain either CDF, CCDF, or PDF plots of the results by moving the cursor to [Plot type], pressing <Enter>, and using the <Up> and <Down> arrow keys to move within the list.

A typical screen plot of the original CDF of a parameter, and the probability of the various quantiles of the original distribution (i.e., quantiles of the original quantiles) subsequent to carrying out the strategy is shown below (Figure 6-1):

Figure 6-1 Effect of Strategy on Parameter

6.2.3 Effect of a Strategy on Performance Results

Version 4.04 does not currently support the ability to evaluate the effect that a strategy has on the performance results. This feature, which was previously available, is currently being modified and will be re-implemented in future versions.

7. RESULTS POST-PROCESSING AND DISPLAY

RIP produces a large volume of output data. The RIP *post-processing module* provides a means of assimilating and comprehending the data. The post-processing module emphasizes use of graphic images and statistical representations of data sets. This chapter describes the use of the post-processor.

7.1 General Information

7.1.1 RIP Data Files

The RIP post-processor synthesizes data contained in several data files. If the user were to create and run a data set titled *test*, the following files would be involved:

- *test.rp* - This is created by the RIP front end which contains the complete RIP input data set.
- *test.btf* - This is the binary transfer file created by the RIP front end as an input file for the RIP back end. Note that an ASCII transfer file can be created using the "-t" switch when running the back end.
- *test.bpf* - This is a binary format file created by the RIP front end when it creates the .btf file. The RIP front-end initially writes the realized values of all stochastic, event and constant parameters to this file. This file is then updated by the back-end to include the final values of all function and table parameters. These parameter values are then read by the post-processor for the display of parameter statistics.
- *test.bsr* - This is a binary output file which contains result statistics (e.g., cumulative releases, peak values).
- *test.btr* - This is a binary output file which contains time history data. This file, along with *test.bsr*, is used to store results for viewing in the post-processor.

In order to view results using the post-processor in the RIP front end, all of these files, with the exception of the .btf file, are required (see Figure 2-9).

7.1.2 Use of Parameters in the Post-Processor

The primary function of the post-processor is to examine relationships between results and system parameters. This is done by viewing many realizations of the system in which the parameters (and hence the results) have different values. For example, one type of analysis allows the user to plot the result (e.g., peak individual dose for a given receptor) against the corresponding value of a particular parameter for each realization.

It is important to understand how the post-processor deals with the various types of parameters:

Constants: Both statistics and time histories of constant parameters can be analyzed in the post-processor. When viewing statistics, the *final value* of the parameter is always presented. Although constants, by definition, consist of a single value, they can be modified by events or by strategy elements. An example of the use of a constant would be to set up a counter to track the number of times a particular event occurred during a realization.

Stochastics: Both statistics and time histories of stochastic parameters can be analyzed in the post-processor. The *final value* of the parameter is saved in the statistics, so that modifications resulting from disruptive events are reflected in the results.

Functions, Tables and Coded Functions: Function, table and coded function parameters can all be analyzed in the post-processor. This includes parameters which are described as explicit functions of time or near-field environmental factors. The final value of all function parameters is saved in the "statistics" result. *If the parameter is a function of the an environmental factor, which can vary among different waste package groups, the variable will always default to the last waste package group.*

Events: Event parameters can be analyzed in the post-processor. The "statistic" value of the event parameter will correspond to the value during the last timestep of each realization. If the event occurred during the final timestep, the parameter will have a value of 1; otherwise, it will be zero.

7.1.3 Entering the Post Processing Module

The user enters the *post-processing module* by selecting [Results] from the top level menu. RIP will then read the output files. The output files will always have the same name (except for the extensions) as the .rp file and must be present within the same directory as the .rp file.

After reading the results file, the following window is displayed:

[■] Repository Integration Program (Rev. 4.04)	
[■] POST PROCESS RIP RESULTS	
Run Desc : Select Output	
Screening Criteria : 5 of 5 Realizations have been selected Result : 0.00E+00 < Release from WP Group # 1 < 0.00E+00 Parameter : No parameter selected	
Select Result Type	: Time History
Select Result Category	: Release from Waste Packages
Select Specific Result	: *Release from WP Group # 1
Select Result Component	: Some
Sort Descending	: Yes
Select Analysis Type	: Time history of Result
Perform Analysis	
F1=ASCII Spreadsheet File F2=ASCII Output File	

7.1.4 Overview of the Post-Processing Window

The post-processing window is divided into several sections, which are used to describe the current model, perform screening operations, select results for viewing and select formats for viewing results. The following paragraphs describe each individual field.

Run Desc - This display field provides a description of the output data set, indicating the number of realizations, the RIP front end version identifier, and the time and date of the front end portion of the run. It can not be edited by the user.

Screening Criteria - The user can specify and analyze subsets of the output data by selecting [Screening Criteria]. For example, the user could choose to examine only those realizations where a *Result* (e.g. release to the accessible environment) or a *Parameter* (e.g. Pathway length), exceeds some threshold value, or is within some specified range. The process for selecting screening criteria is described in more detail in Section 7.2. The *Screening Criteria* display fields show the result and parameter criteria used to create a subset (i.e., screened) data set, and the number of realizations included in this subset.

Since RIP allows the user to save many different types of output data, the post-processor structures the kinds of results that are available for viewing. Five sorting criteria are used to specify the desired type of result: *Result Type*, *Result Category*, *Specific Result*, *Result Component*, and *Analysis Type*. The Result Type field is used to specify whether statistical or time history results will be viewed. Once this has been specified, the user indicates which general type of output (e.g., parameters, release from waste packages) he/she is interested in using the Result Category field. Next, the user indicates which specific output (e.g., parameter, waste package, receptor) to view using the Specific Result field. At this point, for applicable results, the user specifies whether all radionuclides or only certain radionuclides are to be tracked. *Remember that only results selected in the front-end of RIP will be available for viewing in the post-processor.* Finally, Select Analysis Type is used to indicate how the data is to be presented (e.g., distribution, scatter plot, raw data).

Select Result Type - This is an option field that is used to specify whether statistical or time history data is to be viewed. The desired option can be selected by hitting <Enter> and using the <Up> and <Down> arrows to navigate the list.

Select Result Category - This is an option field that is used to indicate the general category of result to be viewed. The options listed here depend upon which results were selected in the front-end and whether "Statistics" or "Time History" was selected in under *Select Result Type*. The desired option can be selected by hitting <Enter> and using the <Up> and <Down> arrows to navigate the list. The available result categories are discussed in Section 7.3.

Select Specific Result - This is an option field that is used to indicate the specific result to be viewed. The options listed here depend upon the option selected under *Select Result Category*. The desired option can be selected by hitting <Enter> and using the <Up> and <Down> arrows to navigate the list. The available results are discussed in Section 7.3.

Select Result Component - This option field is used to indicate which radionuclides are to be viewed, and is only applicable in certain cases. Moving the cursor to this field and hitting <Enter> brings up a list of all radionuclides. (If "Sum" was selected in the front-end, the word "Total" will appear at the top of the list.) The user can scroll the list using the <Up> and <Down> arrows.

The manner in which this field operates depends upon whether "Statistics" or "Time History" is selected. If statistics are being viewed, only a single option on this list can be selected. Hitting <Enter> will select the indicated radionuclide and exit the window. If time history data is being viewed, multiple radionuclides can be plotted. In this case, hitting <Enter> will mark the appropriate radionuclide with a check mark and the window will remain active. Hitting <Esc> will exit the list box and save the selected outputs. The available results are discussed in Section 7.3.

Sort Descending - This field applies only to time history results. Selecting "Yes" sorts the list of radionuclides under "Select Result Component" in descending order, based upon the peak value. Selecting "No" sorts the list in alphabetical order.

Select analysis type - This is an option field which determines the *analysis type*. The desired option can be selected by hitting <Enter> and using the <Up> and <Down> arrows to navigate the list. The available analysis types are described in Section 7.4.

Perform Analysis - When the user selects [Perform Analysis], the *selected analysis* of the *defined result* will be performed on the data meeting the *screening criteria*.

The <F1> key allows the user to create an ASCII spreadsheet file which can be imported into a spreadsheet package. This is discussed further in Section 7.4.3.1. The <F2> key allows the user to create an ASCII output file, which provides a summary of all output parameters and results. This is discussed further in Section 7.4.3.2.

7.2 Screening Criteria

The user enters the *Define Screening Criteria window* (shown below) by selecting [Screening Criteria] from the post-processing window shown above in Section 7.1.

[■] Repository Integration Program (Rev. 4.04)			
[■] POST PROCESS RIP RESULTS			
Run Desc : User's Guide Tutorial			
Screening Criteria : 25 of 25 Realizations have been selected			
Result : 0.00E+00 < Cumulative Release from All WPs < 0.00E+00			
[■] DEFINE SCREENING CRITERIA			
Screening Parameter : A1		Value to use : Realized Value	
Range of Parameter		Actual Range	
MIN : 4	(1.274584)	Number selected	
MAX : 8	(9.904451)	9	
Define Screen Result : Cumulative release to AE			
Range of Result		Actual Range	
MIN : 3447434	(3447434)	Number selected	
MAX : 36816776	(36816776)	24	
9 of 25 realizations have been selected for processing			

The window contains two similar sets of input fields pertaining to the *screening parameter* and the *screening result*.

7.2.1 Defining a Screening Parameter

A screening parameter can be selected by moving to the *Screening Parameter* field and pressing <Enter> for list of available parameters. Having selected a screening parameter, RIP displays the *Actual Range* of values of the screening parameter. The screening range of the parameter is defaulted to the actual range. The user can edit the screening range by entering a new maximum (MAX) or minimum (MIN) value in the appropriate field. Note that the parameter's range can be defined in terms of either the cumulative probability (which ranges from 0 to 1) or the actual realized values. The user chooses between these two choices (using the <PgUp> or <PgDn> toggle keys) in the *Value to use* field. Note that cumulative probability is only applicable for stochastic parameters. For function and event type parameters, the cumulative probability is specified in the post-processor as zero.

Number Selected indicates the number of realizations which meet the screening criteria for the parameter. The number of realizations meeting the screening criteria for both the screening parameter and the screening result (discussed below) is shown on the bottom line of the window.

7.2.2 Defining a Screening Result

A screening result can be defined by selecting [Select screening result]. This brings up the Select Result window shown below:

```

[■] Repository Integration Program (Rev. 4.04 )
[■] POST PROCESS RIP RESULTS
Run Desc : Select Output

Screening Criteria : 6 of 10 Realizations have been selected
Result : 5.80E+01 < Cumulative release to AE < 6.00E+01
[■] DEFINE SCREENING CRITERIA
[■] Select Results

Select Result Category : Cumulative release to AE
Select Specific Result : *Cumulative Release to AE
Select Result Component AC227 58.860847

MIN : 58 (57.15532 ) Number selected
MAX : 59.99788 (59.99788 ) 6

6 of 10 realizations have been selected for processing
    
```

Screening results are selected in the same manner as outputs, with Result Category, Specific Result and Result Component fields. Once the desired result has been selected, hitting <Esc> returns to the main screening menu.

As with the selected screening parameter, RIP displays the *Actual Range* of values of the *screening result*. The screening range of the result is defaulted to the actual range. The user can edit the screening range by entering a new maximum (MAX) or minimum (MIN) value in the appropriate field. Unlike a selected screening parameter, only the *realized values* of a screening result are displayed.

Number selected indicates the number of realizations that meet the screening criteria for the result. The number of realizations meeting the screening criteria for both the screening parameter and the screening result is shown on the bottom line of the window.

7.3 Defining the Result to be Processed

Tables 7.1 and 7.2 summarize the types of results that are available for viewing. Note that only those categories, results and components selected in the front-end will be available for viewing in the post-processor. The individual output categories are discussed in Section 5.5.

Table 7.1 Summary of Statistics Output Options

Select Result Type	Select Result Category	Select Specific Result	Select Result Component
Statistics	Parameters	[Parameter ID] ¹	N/A ²
Statistics	WP Rel.60.113 (Max nuclide)	N/A ³	N/A
Statistics	WP Rel.60.113 (Max release)	N/A	N/A
Statistics	WP Rel.60.113 (Max time)	N/A	N/A
Statistics	WP Rel.60.113 (FF_300)	N/A	N/A
Statistics	WP Rel.60.113 (FF_1000)	N/A	N/A
Statistics	Cum. Release to AE 40 CFR 191	N/A	N/A
Statistics	Cum. Release from Waste Package Groups	WP Group # [n] ⁴	Total or Rn ID ⁵
Statistics	Cumulative Release from all WPs	N/A	Total or Rn ID
Statistics	Cum. Release from WP or Pathways to AE	Release from all WPs or [Pathway ID]	Total or Rn ID
Statistics	Cumulative Release to AE	N/A	Total or Rn ID
Statistics	Cumulative Release from Pathways	[Pathway ID]	Total or Rn ID
Statistics	Release from WP to Pathway	WP Group # [n] to [Pathway ID]	Total or Rn ID
Statistics	Peak Risk by Receptor	[Receptor ID] ⁶	Total or Rn ID
Statistics	Release from one Pathway to Another	Release from [Pathway1 ID] to [Pathway2 ID]	Total or Rn ID
Statistics	Population Risk	N/A	N/A

1 - [Parameter ID] indicates the name of the specific parameter

2 - N/A indicates that there is no Result Component pertaining to this Result Category

3 - N/A indicates that there is only one Specific Result pertaining to this Result Category

4 - [n] indicates the number of the specific waste package group

5 - [Rn ID] indicates the name of the specific radionuclide

6 - [Receptor ID] indicates the name of the specific receptor

Table 7.2 Summary of Time History Output Options

Select Result Type	Select Result Category	Select Specific Result	Select Result Component
Time History	Parameters	[Parameter ID] ¹	N/A ²
Time History	Release from Waste Packages	Release from WP Group # [n] ³	Total or [Rn ID] ⁴
Time History	Release from all WPs	N/A ⁵	Total or [Rn ID]
Time History	Release from WP or Pathway to AE	Release from WP/ Pathway to AE	Total or [Rn ID]
Time History	Total Release to AE	N/A	Total or [Rn ID]
Time History	Release from Pathways	Release from Pathway [Pathway ID]	Total or [Rn ID]
Time History	Release from WP to Pathway	Release from WP Group # [n] to [Pathway ID]	Total or [Rn ID]
Time History	Risk for Receptors	Risk for Receptor [Receptor ID] ⁶	Total or [Rn ID]
Time History	Release from one Pathway to Another	Release from [Pathway1 ID] to [Pathway2 ID]	Total or [Rn ID]
Time History	Mean Risk History for Receptors	[Receptor ID]	Total or [Rn ID]

1 - [Parameter ID] indicates the name of the specific parameter

2 - N/A indicates that there is no Result Component pertaining to this Result Category

3 - [n] indicates the number of the specific waste package group

4 - [Rn ID] indicates the name of the specific radionuclide

5 - N/A indicates that there is only one Specific Result pertaining to this Result Category

6 - [Receptor ID] indicates the name of the specific receptor

7.4 Select Analysis Type

Hitting <Enter> on this field will bring up a list containing a set of available *analysis types*. If "Statistics" is selected as the Result Type, the following selections will appear:

- distribution of result
- contour two parameters versus result
- scatter plot of parameter versus result
- subset of CDF versus original CDF of result
- contribution to mean plot
- correlation matrix
- raw data display

Otherwise, if "Time History" is selected, the following two options are listed:

- raw data display
- time history of result

The analysis types and their respective outputs are described below.

7.4.1 Statistical Outputs

7.4.1.1 Distribution of Result

Distribution of result provides statistical data regarding the selected result. The result statistics are summarized in the Parameter Display Window, shown below:

The *Parameter Display Window* displays the result statistics and can be used to graphically display the distribution in either CDF, PDF or CCDF form. The use of this window is described in detail in Section 4.4.

7.4.1.2 Contour Two Parameters versus Result

While results could be a strong function of a single parameter, the inter-relation between a result and two (or more) parameters is often of greater interest. In RIP, a *contour plot* of the specified result versus any two parameters can be obtained by selecting [Contour Two Parameters versus Result]. When this option is selected, the following window is accessed:

```

[■]-----Repository Integration Program (Rev. 4.04 )-----
[■]-----POST PROCESS RIP RESULTS-----
Run Desc : User's Guide Tutorial
[■]-----PLOT DATA WINDOW-----
Result Desc : Normalized Cumulative Release from All W
Axis type of result : Linear

X-axis Parameter ID : A1          Value to Plot : Realized Value
X-axis type : Linear
Y-axis Parameter ID : FLOW        Value to Plot : Realized Value
Y-axis type : Linear

----- Plot Range -----      ----- Data Range -----
X-axis Parameter : 1             10             1.274584      9.904451
Y-axis Parameter : 50            140            54.37304      138.7005
Z-axis Result      : 3447434      36816776      3447434      36816776

Perform Analysis      F1=Screen Plot (ESC to Exit)
-----F1=ASCII Spreadsheet File-----F2=ASCII Output File-----

```

The result selected in the *define result to be processed* window (Section 7.3) is plotted against two parameters of the user's choice. As with other RIP plot menus, the plot parameters are selected by moving the cursor to the *X-axis and Y-axis Parameter* field, and typing in the parameter name of interest. A list of parameters can be obtained by entering the parameters module (press <Alt>-<P>, then <Alt>-<L>).

The user can specify plotting either *cumulative probability* or *realized* values of the parameters by moving to the *Value to Plot* field and pressing <PgUp> or <PgDn>. Note that cumulative probability only applies for stochastic parameters. The cumulative probability for all function, constant, table and event parameters is specified in the post-processor as zero.

RIP provides default plot scales which the user can override by moving the cursor to the appropriate field and typing in a new plot range value. Log or linear scales can be chosen for all three axes. RIP shows the data ranges for the selected parameters and result to facilitate selection of plot ranges. A screen plot is obtained by pressing <F1> while a hard-copy plot (in HPGL2 format) can be obtained by pressing <F2>. RIP does not actually draw contours, but presents the data in the form of a three-dimensional scatter plot as shown in Figure 7-1.

Figure 7-1 Contour Plot of Two Parameters vs. Result

7.4.1.3 Scatter Plot of Parameter versus Result

A scatter plot provides a powerful visual image of the relationship between the specified result and individual model parameters. The menu for producing a scatter plot is shown below.

```

[■]-----Repository Integration Program (Rev. 4.04 )-----
[■]-----POST PROCESS RIP RESULTS-----
Run Desc : User's Guide Tutorial
[■]-----PLOT DATA WINDOW-----
Result Desc : Normalized Cumulative Release from All W
Axis type for result : Linear

X-axis Parameter ID : AREA      Value to Plot : Realized Value
Axis type for parameter : Linear

----- Plot Range -----      ----- Data Range -----
X-axis Parameter : 0           35           4.004361       31.11682
Y-axis Result      : 3447434    36816776    3447434         36816776
----- F1=Screen Plot (ESC to Exit) -----

Select Analysis Type      : Scatter plot of Parameter vs. Result
Perform Analysis

-----F1=ASCII Spreadsheet File-----F2=ASCII Output File-----
    
```

The result selected in [Define Result to be Processed] (refer to section 7.3) is plotted against the parameter selected in the field *X-axis Parameter ID*. Any defined parameter may be plotted. As always, the user can enter the parameter module to get a listing of parameters by pressing <Alt>-<P> and <Alt>-<L>.

The user can plot either *realized values* or *cumulative probability* of the parameter by moving the cursor to *Value to Plot* and pressing <PgUp> or <PgDn>. Note that cumulative probability only applies for stochastic parameters. The cumulative probability for all function, constant, table and event parameters is specified in the post-processor as zero.

As with other RIP display windows, default plot ranges are chosen by the program. The user can override these ranges by moving the cursor to the appropriate field and entering a new value. Log or linear scales can be chosen for both axes. To aid the user in selecting an appropriate plot range, the actual range of both the parameter and the result are shown. A screen plot is obtained by pressing <F1> while a hard-copy plot (in HPGL2 format) can be obtained by pressing <F2>.

An example of a resulting scatter plot is shown in Figure 7-2.

Figure 7-2 Scatter Plot of Result vs. Parameter

7.4.1.4 Subset of CDF versus Original CDF of Result

When a subset of realizations are selected using the *screening criteria* option (described in Section 7.2), it is often useful to compare a CDF of the data subset with the CDF representing the entire data set. If, for example, the CDF of the realization subset is different from the CDF using all of the realizations, it would imply the screening criteria chosen had an important influence on the result.

This can be done using the *Subset of CDF versus Original CDF of Result* option, which provides access to the following window:

```

[■]-----Repository Integration Program (Rev. 4.04 )-----
[■]-----POST PROCESS RIP RESULTS-----
Run Desc : User's Guide Tutorial
[■]-----PLOT DATA WINDOW-----
Result Desc : Normalized Cumulative Release from All W
Axis type for result : Linear
----- Plot Range ----- Data Range -----
X-axis Result : 3447434 25000000 3447434 36816776
F1=Screen Plot (ESC to Exit)
Select Result Category : Cumulative Release from All WPs
Select Specific Result : Release from all WPs
Select Analysis Type : Subset CDF vs. original CDF of result
Perform Analysis
F1=ASCII Spreadsheet File F2=ASCII Output File
  
```

Plotting is restricted to the CDFs of the data range and its subset. As with other RIP display windows, default scales and titles are supplied by RIP, but can be overridden. A screen plot is obtained by pressing <F1> while a hard-copy plot (in HPGL2 format) can be obtained by pressing <F2>. An example plot is shown in Figure 7-3.

Figure 7-3 Subset of CDF vs. Original CDF of Result

7.4.1.5 Contribution to Mean Plot

The contribution to mean plot is another graphical method of examining the relationship between a result and a parameter. Selecting *contribution to mean* brings up the following window:

Repository Integration Program (Rev. 4.04)	
POST PROCESS RIP RESULTS	
Run Desc : User's Guide Tutorial	
PLOT DATA WINDOW	
Result Desc : Normalized Cumulative Release from All W	
X-axis Parameter ID : AREA	
F1=Screen Plot (ESC to Exit)	
Select Result Category	: Cumulative Release from All WPs
Select Specific Result	: Release from all WPs
Select Analysis Type	: Contribution to Mean Plot
Perform Analysis	
F1=ASCII Spreadsheet File	F2=ASCII Output File

The user selects the parameter to be plotted (*X-axis Parameter ID*), and presses <F1> to obtain a screen plot or <F2> to obtain a hard-copy plot (in HPGL2 format).

The contribution to mean is a plot of the CDF of a specified parameter (plotted along the X-axis) versus the fraction of the total result. The curvature (i.e., slope) of the line plotted is an indication of the dependence of the result on the parameter. For example, if the line is near vertical at low values of the parameter and near horizontal at high values of the parameter, this would indicate that the result (e.g., waste package release) is sensitive to the parameter when the value of the parameter is small. Conversely, if the line is near horizontal at low values of the parameter and near vertical at high values of the parameter, this would indicate that the result is sensitive to the parameter when the value of the parameter is large. In the example shown in Figure 7-4, the slope of the line is uniform throughout the data range, indicating that the result is insensitive to the parameter (in this case, the catchment area).

Figure 7-4. Contribution to Mean Plot

7.4.1.6 Correlation Matrix

When correlation matrix is selected, a statistical correlation analysis is conducted on all stochastic parameters and all selected results to determine how particular results are correlated against particular parameters.

RIP can compute two different types of correlation. The first, referred to as the *correlation coefficient*, is computed as follows:

$$\rho = \frac{\sum_{i=1}^n (p_i - m_p)(r_i - m_r)}{\sqrt{\sum_{i=1}^n (p_i - m_p)^2 \sum_{i=1}^n (r_i - m_r)^2}} \quad (7.1)$$

where:

- ρ = the correlation coefficient;
- n = the number of data points (realizations);
- p_i = value of parameter for realization i ;
- r_i = value of result for realization i ;
- m_p = mean value of parameter;
- m_r = mean value of result;

The correlation coefficient takes on a value between -1 and 1, 1 being a perfect positive correlation, -1 being a perfect negative correlation. (If the standard deviation of a parameter or a result is 0, RIP sets the correlation coefficient to zero.)

Note that the correlation coefficient as defined here provides a measure of the *linear* relationship between two variables. Furthermore, it may be affected by a few aberrant pairs (a good alignment of a few extreme pairs can dramatically improve an otherwise poor correlation coefficient; likewise, an otherwise good correlation could be ruined by the poor alignment of a few extreme pairs).

To overcome these problems, the correlation coefficient can be supplemented by another measure, the *rank correlation coefficient*. The rank correlation coefficient is computed using the same equation (7.1), in which the ranks of the data values are used rather than the actual values:

$$\rho_{\text{rank}} = \frac{\sum_{i=1}^n (Rp_i - m_{Rp})(Rr_i - m_{Rr})}{\sqrt{\sum_{i=1}^n (Rp_i - m_{Rp})^2 \sum_{i=1}^n (Rr_i - m_{Rr})^2}} \quad (7.2)$$

where Rp_i and Rr_i are the ranks (from 1 to n) of the parameter value and result, respectively, for realization i , and m_{Rp} and m_{Rr} are the means of the ranks of the parameter and the result, respectively. In RIP, the ranks of equal values are the same. For example, if the lowest two realizations of a parameter were the same, their ranks would both be 1.5 (the mean of 1 and 2), with the third lowest parameter being assigned a rank of 3.

After choosing to compute a correlation matrix, the user is asked whether to compute the correlation coefficient or the rank correlation coefficient. Depending on the number of parameters and realizations, the subsequent analysis could be relatively time-consuming. When the analysis is complete, a matrix of correlation coefficients is produced for all parameters versus all results as shown below:

Repository Integration Program (Rev. 4.04)				
POST PROCESS RIP RESULTS				
CORRELATION MATRIX				
Parameter ID	Mean Value	Result Normalized	Cum. Release from Waste Packa	STANDARD
AMTRX	5.0843E+01	-0.281		
AREA	1.3311E+00	-0.955		
CATCH	1.0391E+03	0.693		
DISS	3.4127E-02	0.850		
FLOW	1.9502E+00	0.702		
JUNK	9.8308E+00	0.765		
MODE1	3.6919E+03	0.578		
MODE2	5.3129E+03	0.783		
PLEN2	7.6120E+02	-0.680		
POROS	5.2225E-01	-0.519		
PLEN1	1.5224E+03	-0.680		

F1=SCROLL ROWS UP F2=SCROLL ROWS DOWN

The first column (immediately adjacent to the parameter name) is the mean of the realized values (or the mean of the ranks) of the parameter for the particular data set or subset (if it was screened) which was chosen. Either "Standard" or "Rank" is displayed in the upper right hand corner of the window to remind the user of the type of correlation displayed.

If there are sufficient parameters or results such that the entire matrix cannot be completely displayed on a single screen, the user can scroll through the results using the function keys <F1> to <F4>, as indicated at the bottom of the screen.

7.4.1.7 Raw Data Display

The realized values or cumulative probability of all parameters and realized values of results are shown when *raw data display* is selected. An example of a raw data display is shown below:

Repository Integration Program (Rev. 4.04)						
POST PROCESS RIP RESULTS						
RAW DATA DISPLAY						
REAL NO	Realized Value A1	PARAMETERS FLOW	KD	OMEGA	SORT RES1	RESULTS RES2
2	6.07E+00	9.43E+01	1.00E+00	1.52E-03	1.80E+07	1.00E+00
3	5.73E+00	1.28E+02	1.00E+00	5.03E-04	2.30E+07	1.00E+00
7	4.58E+00	1.22E+02	1.00E+00	5.67E-04	1.76E+07	1.00E+00
16	5.74E+00	9.89E+01	1.00E+00	9.22E-04	1.78E+07	1.00E+00
17	4.43E+00	5.44E+01	1.00E+00	7.57E-04	7.57E+06	1.00E+00
19	4.03E+00	1.25E+02	1.00E+00	1.59E-03	1.58E+07	1.00E+00
20	4.98E+00	8.24E+01	1.00E+00	1.67E-03	1.29E+07	1.00E+00
23	6.61E+00	1.23E+02	1.00E+00	1.51E-03	2.56E+07	1.00E+00
25	7.45E+00	1.12E+02	1.00E+00	5.51E-04	2.62E+07	1.00E+00

F1=SCROLL ROWS UP F2=SCROLL ROWS DOWN F3=SCROLL PARS LEFT F4=SCROLL PARS RIGHT F5=TOGGLE PARS F6=ORDER COLS

The user can scroll through the data by pressing the function keys (<F1> to <F4>) as noted at the bottom of the screen. The user can toggle between displaying *realized values* or *cumulative probability* of parameters by pressing <F5>. Note that cumulative probability only applies for stochastic parameters. The cumulative probability for all function, constant, table and event parameters is specified in the post-processor as zero.

Pressing <F6> allows the user to select four specific parameters for display (note: use of this option disables scrolling parameters left or right with the <F3> and <F4> keys).

The user can sort the realizations as a function of any result by moving the cursor to *SORT* and pressing enter (this will call up a Sort window where sorting criteria are entered). Moving the cursor to *RES1* or *RES2* and pressing <Enter> will bring up a window with a description of the result.

7.4.2 Time History Outputs

7.4.2.1 Time History of Result

RIP provides the option to save time history information for individual realizations for both results and individual parameters. RIP stores the time history data for results based upon the following criteria.

1. If any risk time histories are selected (i.e., either total risk to a receptor or mean risk to a receptor), the five realizations which contain the highest peak risk to any receptor at any time step are saved.
2. If the no risk histories are selected and the simulation is run using only the waste package model (i.e., pathways are not simulated), then the five realizations which contain the highest cumulative release from waste packages are saved.
3. Otherwise, the five realizations which result in the greatest normalized release to the AE (as defined under 40 CFR 191.13) are saved.

Additionally, time histories can be viewed any parameter, although only the first realization is saved. Time histories are saved for all parameters for which this option is selected within the parameters database in the RIP front-end.

Time histories of results can be displayed by selecting [Time history of result]. The user is first asked which time history (of the five) is to be plotted, as shown below:

```

[ ] Repository Integration Program (Rev. 4.04 )
[ ] POST PROCESS RIP RESULTS
Run Desc : Select Output

Screening Criteria : 400 of 400 Realizations have been selected
Result : Release from WP Group # 1
Parameter : No parameter selected

Select Result Type : Time History
Select Result C [ ] SELECT TIME HISTORY
The top 5 time histories [ ] ved
Select time history to plot : 47
5
156
239
12
Select Specific
Select Result Component Some
Sort Descending Yes

Select Analysis Type : Time history of Re
Perform Analysis
F1=ASCII Spreadsheet File F2=ASCII Output File
  
```

Note that time histories are listed in descending order, using the selection criteria defined above. As shown in the example above, realizations 5, 12, 47, 156 and 239 had the highest values, with realization 47 having the highest, realization 5 the second highest, and so on.

Having selected a time history, the user presses <Esc> to move to the *plot data window* shown below:

```

[ ] Repository Integration Program (Rev. 4.04 )
[ ] POST PROCESS RIP RESULTS
Run Desc : User's Guide Tutorial
[ ] PLOT DATA WINDOW
Result Desc : Release from all WPs
Axis type for result : Linear
X-axis type for time : Linear
Time Point file name : timehist.dat

----- Plot Range ----- Data Range -----
X-axis Time : 0 10000 0 10000
Y-axis Result : 0 2500 0 2252.389

F1=Screen Plot F3=Time points to file ESC=Cancel

Select Analysis Type : Time history of Result
Perform Analysis
F1=ASCII Spreadsheet File F2=ASCII Output File
  
```

RIP selects a default plot range for the X- and Y-axis, but this can be overridden by the user by moving the cursor to the appropriate field and entering a new plot range value. Log or linear scales can be chosen for both axes. As with other RIP plotting windows, the range of realized values is shown to aid the user in selecting a plot range. A screen plot is obtained by pressing <F1>. An example of a time history plot is shown in Figure 7-5.

Figure 7-5 Time History Plot

The <F3> key creates an ASCII file of the time history, which can then be imported to other software packages (e.g., spreadsheets). The user specifies the name of the ASCII file in the input window (the default name being timehist.dat). Note that this time history is saved as the value per timestep (not per unit time).

Risk time history plots are created in the same manner. If mean risk histories are chosen, the user has the option to plot either: 1) the total mean risk (summed over all radionuclides); 2) the mean risk from one or more specific radionuclides (superimposed on the same plot). An example of mean risk for multiple radionuclides is shown in Figure 7-6.

Figure 7-6 Time History of Mean Risk by Radionuclide

Note that RIP calculates and plots the standard deviation of risk, along with the mean risk (if "total" or a single radionuclide is selected). This gives an indication of the uncertainty involved. Note that when saving one of these mean risk plots to an ASCII file (using the <F3> key), both the mean risk and the standard deviation are written.

When results vary from realization to realization by orders of magnitude, the mean risk history will tend to be dominated by the high realizations. Furthermore, adding and subtracting a standard deviation to the mean risk curve is likely to be less meaningful, as the distribution of uncertainty would not be expected to be symmetric. Figure 7.7 shows a mean risk history with standard deviation bands.

Figure 7-7 Time History Plot of Mean Risk to Receptor

Additionally, time history plots can also be viewed for parameters. Parameters for which time history information is saved are indicated in the front-end parameters database by selecting "yes" in the "Save Time History" field. Note, however, that only the first realization is saved for each parameter. Figure 7-8 shows a time history plot of a parameter. In this instance, the parameter is a counter used to track the occurrence of a particular event.

Figure 7-8 Time History Plot of a Parameter

7.4.2.2 Raw Data Display

As with statistics, it is possible to view raw data of a time history result. In this case, the value of the parameter or result is saved at each time step. This is useful when more precision is required than can be observed from the time history plots.

As with time history plots, the desired realization number must be indicated (the five realizations with highest normalized cumulative releases are saved). After this is done, the time history data points appear in the following window:

Repository Integration Program (Rev. 4.04)						
POST PROCESS RIP RESULTS						
TIME	SORT		TIME HISTORY DATA			
STEP	RES1	RES2	RES0	RES0	RES0	RES0
100	1.16E+02					
200	1.26E+02					
300	1.36E+02					
400	1.46E+02					
500	1.56E+02					
600	1.66E+02					
700	1.76E+02					
800	1.86E+02					
900	1.96E+02					
1000	2.06E+02					
1100	2.16E+02					
1200	2.26E+02					
1300	2.36E+02					
1400	2.46E+02					
1500	2.56E+02					
1600	2.66E+02					
1700	2.76E+02					

F1=SCROLL UP F2=SCROLL DOWN F3=SCROLL RESULTS LEFT F4=SCROLL RESULTS RIGHT

The column at the far left displays the time points and the second column from the left displays the result value at the corresponding time. Moving the cursor to RES1 and hitting <Enter> will display the result type that is shown. Note that, for all categories except risk, the data are presented in terms of value per timestep, not per unit time. However, for risk categories, the raw data values are reported on a per unit time basis since risk is not generally considered to be cumulative.

Moving the cursor to the SORT field and hitting <Enter> brings up a dialog box giving the option to sort the results in either ascending or descending order.

7.4.3 Output Data Files

7.4.3.1 ASCII Spreadsheet File

In some cases, it may be useful to analyze results generated by RIP using a separate statistical analysis software package. To facilitate this, RIP provides the option of writing results to a standard output file that can subsequently be read into such a package. This is done by hitting the <F1> key from the main result post-processing window. The user will be prompted for a filename.

The top of the ASCII file contains header information containing the following:

- 1) the run description;
- 2) the selected result;
- 3) the manner in which the results in the file have been screened.

This is followed by a blank line.

The results are then printed as rows and columns. The first row contains the parameter names. The last column of the first row is titled "result", and refers to the selected result identified in the header. Each subsequent row lists the parameter values and the result for a particular realization. An example of this output file is shown below:

Run description : User's Guide Tutorial

The selected result is Cumulative Release from All WPs

Screening criteria : 10 of 10 realizations selected

Screening parameter : No parameter selected

Screening result : Cumulative Release from All WPs ; 0.00E+00 < val < 0.00E+0

A1	FLOW	KD	OMEGA	PI	EVENT	AREA	TMFFUN	Result
3.2950275	295.49963	1	0.0009912	3.1417	1	10.351987	200	8.694864E+6
1.0800925	275.49298	1	0.0004109	3.1417	1	3.3933268	200	2.578599E+6
6.8375382	277.35803	1	0.0013236	3.1417	1	21.481494	200	1.648409E+7
3.9477272	295.21652	1	0.0014571	3.1417	1	12.402574	200	1.040315E+7
1.1752346	318.71942	1	0.0015182	3.1417	1	3.6922345	200	3.44409E+6
7.2544265	274.74249	1	0.0005026	3.1417	1	22.791231	200	1.725071E+7
1.4028529	278.20605	1	0.0015606	3.1417	1	4.4073429	200	3.396978E+6
4.3782644	269.99438	1	0.0013772	3.1417	1	13.755193	200	1.01501E+7
8.0264568	306.01181	1	0.002804	3.1417	1	5.21677	200	1.22401E+7
1.3967664	277.7182	1	0.0011685	3.1417	1	4.3887712	200	3.17367E+6

This file can subsequently be imported into a spreadsheet, or a simple program can be written to convert it to any desired format.

7.4.3.2 ASCII Output file

For a more detailed summary of output data, the <F2> key can be used to create an ASCII output file. This file contains extensive labels and formatting for easier viewing of output data. The values of all saved parameters and results are listed for each realization. Printing this file provides a comprehensive summary of the results generated by the simulation; however, if many parameters or many realizations are used, this file can become quite long. An example of an ASCII output file is presented in Appendix F of the RIP User's Guide.

8. REFERENCES

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APPENDIX A

STOCHASTIC PARAMETER DISTRIBUTIONS

This appendix is divided into two parts. In the first (A-1), the mathematical forms for the various stochastic parameter distributions available within RIP are described. In the second part (A-2), the actual input windows for the various distributions are presented and discussed.

A-1. MATHEMATICAL FORMS OF AVAILABLE PROBABILITY DISTRIBUTIONS

As discussed in Section 4.3.3, RIP provides the following distributions:

- Normal
- Log-Normal
- Uniform
- Log-Uniform
- Triangular
- Log-Triangular
- Cumulative
- Discrete
- Poisson
- Beta
- Gamma
- Weibull
- Binomial
- Boolean

The appropriate parameters, the probability density function (pdf), the cumulative distribution function (cdf), and the mean and variance for each distribution are presented below.

A-1.1 Normal Distribution

The normal distribution is specified by a mean (μ) and a standard deviation (σ). The linear normal distribution is a bell shaped curve that is typically used for describing characteristics of a population.

Pdf: $f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$

cdf: No closed-form solution

mean: μ

variance: σ^2

A-1.2 Log-Normal Distribution

The log-normal distribution is used when the *logarithm* of the random variable is described by a normal distribution. The distribution is specified by the exponentiated mean of the logarithms (μ), and the standard deviation of the log of the distribution (σ).

$$\text{pdf: } f(x) = \frac{1}{x \ln(10) \sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \left(\frac{\ln(x) - \mu}{\sigma \ln(10)} \right)^2}, \quad x > 0$$

cdf: No closed-form solution

$$\text{mean: } \mu = e^{\left[\ln(\mu) + \frac{C_1}{2} \right]}$$

$$\text{variance: } \sigma^2 = e^{\left[\ln(\mu) + \frac{C_1}{2} \right]} \cdot \left[\frac{\ln(e^{C_1})}{2} \right]$$

$$\text{where: } C_1 = [\ln(10)]^2$$

A-1.3 Uniform Distribution

The uniform distribution is specified by a minimum value (a) and a maximum value (b). Each point between the endpoints has an equal likelihood of occurring. This distribution is used when a quantity varies uniformly between two values, or when only the endpoints of a quantity are known.

$$\text{pdf:} \quad f(x) = \begin{cases} \frac{1}{b-a}, & a \leq x \leq b \\ 0, & \text{otherwise} \end{cases}$$

$$\text{cdf:} \quad F(x) = \begin{cases} 0, & x < a \\ \frac{x-a}{b-a}, & a \leq x \leq b \\ 1, & x > b \end{cases}$$

$$\text{mean:} \quad \mu = \frac{b+a}{2}$$

$$\text{variance:} \quad \sigma^2 = \frac{(b-a)^2}{12}$$

A-1.4 Log-Uniform Distribution

The log-uniform distribution is used when the *logarithm* of the random variable is described by a uniform distribution. The minimum (a) and maximum (b) values are specified in linear space.

$$\text{pdf:} \quad f(x) = \begin{cases} \frac{1}{x \left[\ln\left(\frac{b}{a}\right) \right]}, & a \leq x \leq b \\ 0, & \text{otherwise} \end{cases}$$

$$\text{cdf:} \quad F(x) = \begin{cases} 0, & x < a \\ \frac{\ln\left(\frac{x}{a}\right)}{\ln\left(\frac{b}{a}\right)}, & a \leq x \leq b \\ 1, & x > b \end{cases}$$

$$\text{mean:} \quad \mu = \frac{b - a}{\ln\left(\frac{b}{a}\right)}$$

$$\text{variance:} \quad \sigma^2 = \frac{b^2 - a^2}{2 \ln\left(\frac{b}{a}\right)} - \frac{(b - a)^2}{\left[\ln\left(\frac{b}{a}\right) \right]^2}$$

A-1.5 Triangular Distribution

The triangular distribution is specified by a minimum value (a), a most likely value (b), and a maximum value (c).

$$\text{Pdf: } f(x) = \frac{2(x-a)}{(b-a)(c-a)}, \quad a \leq x \leq b$$

$$\frac{2(c-x)}{(c-b)(c-a)}, \quad b \leq x \leq c$$

$$\text{cdf: } F(x) = 0, \quad x < a$$

$$\frac{(x-a)^2}{(b-a)(c-a)}, \quad a \leq x \leq b$$

$$1 - \frac{(c-x)^2}{(c-b)(c-a)}, \quad b < x \leq c$$

$$1, \quad x > c$$

$$\text{mean: } \mu = \frac{a + b + c}{3}$$

$$\text{variance: } \sigma^2 = \frac{a^2 + b^2 + c^2 - ab - ac - bc}{18}$$

A-1.6 Log-Triangular Distribution

The log-triangular distribution is used when the *logarithm* of the random variable is described by a triangular distribution. The minimum (a), most likely (c), and maximum (b) values are specified in linear space.

$$\text{pdf: } f(x) = \begin{cases} \frac{2 \ln\left(\frac{x}{a}\right)}{\ln\left(\frac{b}{a}\right) \ln\left(\frac{c}{a}\right)}, & a \leq x \leq c \\ \frac{2 \ln\left(\frac{b}{x}\right)}{\ln\left(\frac{b}{a}\right) \ln\left(\frac{b}{c}\right)}, & c \leq x \leq b \\ 0, & \text{otherwise} \end{cases}$$

$$\text{cdf: } F(x) = \begin{cases} 0, & x < a \\ \frac{\left[\ln\left(\frac{x}{a}\right)\right]^2}{\ln\left(\frac{b}{a}\right) \ln\left(\frac{c}{a}\right)}, & a \leq x \leq c \\ 1 - \frac{\left[\ln\left(\frac{b}{x}\right)\right]^2}{\ln\left(\frac{b}{a}\right) \ln\left(\frac{b}{c}\right)}, & c < x \leq b \\ 1, & x > c \end{cases}$$

$$\text{mean: } \mu = \frac{2}{d_1} \left\{ a + c \left[\ln\left(\frac{c}{a}\right) - 1 \right] \right\} + \frac{2}{d_2} \left\{ b + c \left[\ln\left(\frac{c}{b}\right) - 1 \right] \right\}$$

$$\text{variance: } \sigma^2 = \frac{2}{d_1} \left\{ \frac{a^2}{4} + \frac{c^2}{2} \left[\ln\left(\frac{c}{a}\right) - \frac{1}{2} \right] \right\} + \frac{2}{d_2} \left\{ \frac{b^2}{4} + \frac{c^2}{2} \left[\ln\left(\frac{c}{b}\right) - \frac{1}{2} \right] \right\} - \mu^2$$

where:

$$d_1 = \ln\left(\frac{b}{a}\right) \ln\left(\frac{c}{a}\right)$$
$$d_2 = \ln\left(\frac{b}{a}\right) \ln\left(\frac{b}{c}\right)$$

- **Disagreement** Multiple assessments are determined where convergence or consensus on a single assessment is not possible (e.g., owing to major differences of opinion).

In general, convergence is generally most desirable, as it is most defensible, but may be difficult to achieve. Agreed consensus, i.e., with the concurrence of the group, is slightly less defensible but also less difficult to achieve. Forced consensus, without concurrence of the group, may be difficult to defend but is very simple. Disagreement may be difficult to use, as it is non-unique, but is defensible.

Techniques available for resolving differences of opinion amongst a group of individual assessors can be categorized in terms of "mechanical aggregation" and "behavioral procedures":

- **Mechanical aggregation** of individual assessments is a relatively simple approach to achieving at least forced consensus, and involves applying a mathematical formula or procedure to combine the various individual probability distributions^{16,17}. If the individuals in the group agree to the resulting distribution, then agreed consensus (and possibly convergence) can be achieved. In general, mechanical aggregation techniques are most useful when the means, rather than the variances, of the individual probability distributions differ. Also, mechanical aggregation techniques can be used when a single distribution is required, but the scenario/parameter in question is not significant enough to warrant large amounts of effort to achieve convergence or agreed consensus.

The various forms of mechanical aggregation include the following²:

- **Averaging**, which is the simplest mechanical aggregation technique, involves simply averaging the individuals' probabilities for each possible value. Several empirical studies^{18,19} have shown that averaged probabilities are often superior to individual assessments. As an example, if one individual assessed an 80% probability of the average large-scale hydraulic conductivity (log) being less than -3.5 and the other individual in the group assessed a 60% probability, then the group average would be a 70% probability.
- **Group statistics**, which is a somewhat more rigorous treatment, involves determining the group's distribution of opinions regarding the probability for each value, thereby developing a "fuzzy" assessment or an assessment which corresponds to a given level of conservatism for the group. More complete statistical methods are available that incorporate dependence among variables and experts' and least squares or partitioning methods²⁰. As an example, the statistics of the group members' opinions of the probability of the average large-scale hydraulic conductivity (log) being less than -3.5 could be determined and used.
- **Weighting methods**, which are elaborations on either averaging or group statistics, involve the weighting of individual assessments by an external

procedure to incorporate biases or differing levels of expertise among the individual assessors, similar to individual calibrated assessments. There are essentially two weighting procedures:

- * "calibration exercise", in which the natural biases and tendencies of the individual assessors are evaluated and mitigated through 1) the administration of a series of general questions to determine each assessor's ability to make correct assessments, and 2) the determination and application of weighting factors for each assessor to reflect that assessor's ability (relative to the other assessors) to make correct assessments; and
 - * "peer ratings", in which each of the individual assessor's relative ability to make correct assessments is assessed subjectively by peers, although such a subjective assessment may itself introduce additional biases.
- **Behavioral procedures** can be used to attempt to develop convergence or at least agreed consensus, and involve interaction among the individuals in the group, which allows for the explicit identification and resolution of differences of opinion. Although there is evidence that such interaction results in better assessments^{21,22} and that the results are generally more defensible, because the group agrees on a given distribution, behavioral procedures tend to entail significantly more effort, because the various individual assessors must be involved. Such behavioral procedures are necessary when at least agreed consensus (or disagreement) is required (i.e., for significant parameters), and are especially useful when the differences between the individual assessments are large.

As summarized in Table 1, the various forms of behavioral procedures include the following²:

- **Open forum** is a very informal means of achieving consensus and does not require prior individual assessments. The group attempts to achieve convergence or agreed consensus by open discussion of whatever each individual deems important to resolving the problem. A major limitation of this method is that the result can be distorted by the dynamics of the group, such as domination by an individual because of status or personality²³. For example, the persuasiveness of a vocal individual or the desire of some individuals to avoid dissension may distort the results. Other potential limitations to this method are the same as for the development of individual assessments through the informal solicitation of expert opinion, i.e., poor quantification of uncertainty, uncorrected biases, unspecified assumptions, and poor problem definition. The method is also limited by the credibility of the group members.

A-1.9 Poisson Distribution

The Poisson distribution is specified by a rate (R). It is often used to model the number of individual events that occur in a given unit of time, such as the number of earthquakes or volcanic eruptions over a specified period of time.

pdf: $f(x) = \frac{e^{-R} R^x}{x!}$

cdf: $F(x) = e^{-R} \sum_{i=0}^x \frac{R^i}{i!}$

mean: $\mu = R$

variance: $\sigma^2 = R$

A-1.10 Beta Distribution

The beta distribution is specified by a mean (T), a standard deviation (I), a minimum value (a), and a maximum value (b).

$$\text{pdf: } f(x) = \frac{1}{a-b} \beta(R, T) \left(\frac{x-a}{b-a} \right)^{R-1} \left(1 - \frac{x-a}{b-a} \right)^{T-R-1}$$

$$\text{where: } A = \frac{\mu - a}{b - a}$$

$$B = \frac{\sigma}{(b-a)^2}$$

$$T = \frac{A+B}{A-B}$$

$$R = TA$$

$\beta(x, y)$ is the B function

cdf: No closed form

mean: T

variance: I^2

The beta distribution is sometimes defined using the arguments I and θ . These parameters are related to T , I , a and b as follows:

$$\alpha = \left[\frac{X^2}{Y^2} (I - X) \right] - (I + X)$$

$$\beta = \frac{\alpha + 1}{X} - (\alpha + 2)$$

where $X = (T - a)/(b - a)$ and $Y = I/(b - a)$.

A-1.11 Gamma Distribution

The gamma distribution is specified by a mean (T) and a standard deviation (I).

$$\text{pdf: } f(x) = \frac{\lambda(\lambda x)^{k-1} e^{-\lambda x}}{\Gamma(k)}$$

$$\text{cdf: } F(x) = \frac{\Gamma(k, \lambda x)}{\Gamma(k)}$$

$$\text{where: } k = \frac{\mu^2}{\sigma^2}$$

$$\lambda = \frac{\mu}{\sigma^2}$$

$$\begin{aligned} \Gamma(k, x) &= \text{Incomplete Gamma Function} \\ \Gamma(x) &= \text{Gamma Function} \end{aligned}$$

$$\text{mean: } T$$

$$\text{variance: } I^2$$

A-1.12 Weibull Distribution

The weibull distribution is specified by a minimum value (M), a scale parameter (θ), and a slope or shape (I). This distribution is often used to model the lifetime of an item for reliability studies.

$$\text{pdf: } f(x) = \frac{\alpha}{\beta - \varepsilon} \left(\frac{x - \varepsilon}{\beta - \varepsilon} \right)^{\alpha-1} e^{-\left(\frac{x - \varepsilon}{\beta - \varepsilon} \right)^{\alpha}}, \quad x \geq \varepsilon > 0$$

$$\text{cdf: } F(x) = 1 - e^{-\left(\frac{x - \varepsilon}{\beta - \varepsilon} \right)^{\alpha}}$$

$$\text{mean: } \frac{\beta - \varepsilon}{\alpha} \Gamma\left(\frac{1}{\alpha}\right)$$

$$\text{variance: } \frac{(\beta - \varepsilon)^2}{\alpha} \left\{ 2\Gamma\left(\frac{2}{\alpha}\right) - \frac{1}{\alpha} \left[\Gamma\left(\frac{1}{\alpha}\right) \right]^2 \right\}$$

A-1.13 Binomial Distribution

The binomial distribution is specified by a batch size (N) and a probability of occurrence (P). This distribution can be used to model the number of parts that failed from a given set of parts, where N is the initial number of parts and P is the probability of the part failing.

$$\text{pdf: } f(x) = \binom{N}{x} P^x (1-P)^{N-x}$$

$$\text{cdf: } F(x) = \sum_{i=0}^x \binom{N}{i} P^i (1-P)^{N-i}$$

$$\text{mean: } NP$$

$$\text{variance: } NP(1-P)$$

A-1.14 Boolean Distribution

The Boolean (or logical) distribution requires a single input: the Probability of being True, P . The distribution takes on one of two values: 0 (false) or 1 (true).

pdf:	$f(x) =$	$1-P,$	$x=0$
		$P,$	$x=1$
cdf:	$F(x) =$	$1-P,$	$x=0$
		$1,$	$x=1$
mean:		$0,$	$P < 0.5$
		$1,$	$P \geq 0.5$

A-2. RIP INPUT WINDOWS FOR STOCHASTIC DISTRIBUTIONS

The input windows for the distributions described in the previous sections are discussed below. Note that as discussed in Section 4.3.3, every type of stochastic parameter input window has a "Sampling Bias" input field, which refers to the amount of importance sampling (or biasing) which is to be used when sampling the distribution. This is discussed in detail in that section and will not be discussed further here.

Except where specifically noted below, data fields for the various distributions may be specified as constants, other stochastics, or functions.

A-2.1 Normal Distribution

The normal distribution takes two forms: linear or log. Once a normal distribution is selected, the user toggles between linear and log using the <F3> key. The linear and log input windows for the normal distribution are slightly different. The linear normal distribution input window is shown below:

```

[■]-----Repository Integration Program (Rev. 4.04 )-----
General      PA Model      Strategy Model      Results
[■]-----Parameter Editing-----
Identifier : STOCH1.                      Parameter No. : 31 of 39
Description:
Parameter Type : Stochastic
( 0 )

Save Time [■]-----NORMAL DISTRIBUTION-----
Edit Param Sampling Bias : No Bias          F1=Prev type
Affects    Mean : 0                      (Constant ) F2=Next type
           S.D. : 0                      (Constant ) F3=Log/linear
           F5=Truncated

[Function]

F1=Prev Param  F2=Next Param  F3=Add Param  F4=Delete Param
F5=Find Param  F6=Print Summary F7=Display Dist. F8=Expected Value
F9=Strategy    F10=Bayesian update (Current update level=0 )
  
```

```

[■]-----Repository Integration Program (Rev. 4.04 )-----
General      PA Model      Strategy Model      Results
[■]-----Parameter Editing-----
Identifier : STOCH1.                      Parameter No. : 31 of 39
Description:
Parameter Type : Stochastic
Normal : Mean : 10, S.D. : 5, Min. : 0, Max. : 20 )

Save Time [■]-----TRUNCATED NORMAL DISTRIBUTION-----
Edit Param Sampling Bias : No Bias          F1=Prev type
Affects    Mean : 10                      (Constant ) F2=Next type
           S.D. : 5                      (Constant ) F3=Log/linear
           Min : 0                      (Constant ) F5=Non-
           Max : 20                      (Constant ) Truncated

[Function]

F1=Prev Param  F2=Next Param  F3=Add Param  F4=Delete Param
F5=Find Param  F6=Print Summary F7=Display Dist. F8=Expected Value
F9=Strategy    F10=Bayesian update (Current update level=0 )
  
```

The input is straightforward and consists simply of the mean and the standard deviation. The user can choose between Truncated or Non-Truncated using the <F5> key, as shown on the previous page:

The window for the log-normal distribution is similar and is shown below:

```

[■]-----Repository Integration Program (Rev. 4.04 )-----
      General      PA Model      Strategy Model      Results
[■]-----Parameter Editing-----
Identifier : Stoch1      Parameter No. : 31 of 39
Description:
Parameter Type : Stochastic
( log- Normal : Mean = 1000, geometric S.D. = 2 )
Save Time [■]-----LOG-NORMAL DISTRIBUTION-----
Edit Param
[Affects]   Sampling Bias : 0 Bias
[Function]   Geometric-Mean: 1000      (Constant )
              Geometric-SD : 2        (Constant )
              True Mean : 1071.537
              True S.D. : 998.6275
              F5=Truncated
F1=Prev Pa
F5 Find Param  F6 Print Summary  F7 Display Dist.  F8=Expected Value
F9 Strategy    F10=Bayesian update (Current update level 0 )
  
```

Log-normal distributions can be entered in two ways: 1) by entering the "Geometric Mean" and the "Geometric S.D."; or 2) by entering the "True Mean" and the "True S.D." The <F4> key is used to toggle between these two options. When one option is chosen, the other set of parameters are computed internally by RIP and cannot be edited.

With regard to a set of data points, the "Geometric Mean" is equal to the exponentiated mean of the logs (i.e., 10^X , where X is equal to the mean value of the logarithms of the data points). In previous versions, this field was defined identically, but was referred to as the "Log-Mean".

With regard to a set of data points, the "Geometric S.D." is the equivalent to the exponentiated S.D. of the logs (i.e., 10^Y , where Y is equal to the standard deviation of the logarithms of the data points). *Note that in versions of RIP prior to 4.00, this field was defined differently. In particular, instead of entering 10^Y , the user entered Y. When reading old data files (i.e., previous to 4.00), RIP will automatically convert any existing log-normal distributions to be consistent with the new manner in which the input fields are defined.*

The "True Mean" and the "True S.D." refer to the true (arithmetic) mean and S.D. (i.e., in linear space).

The <F5> key can be used to specify minimum and maximum bounds.

A-2.2 Uniform Distribution

The uniform distribution takes two forms: linear or log. Once a uniform distribution is selected, the user toggles between linear and log using the <F3> key. The linear and log input windows for the uniform distribution are identical (except for the field which identifies the window as linear or log):

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Parameter Editing		Parameter No. : 31 of 39	
Identifier : STOCH1			
Description:			
Parameter Type : Stochastic			
(0)			
Save Time	UNIFORM DISTRIBUTION		
Edit Param	Sampling Bias : No Bias	F1=Prev type	
(Affects	log	F2=Next type	
	Lower bound: 0 (Constant)	F3=Log/Linear	
(Function	Upper bound: 100 (Constant)		
F1=Prev Param F2=Next Param F3=Add Param F4=Delete Param			
F5=Find Param F6=Print Summary F7=Display Dist. F8=Expected Value			
F9=Strategy F10=Bayesian update (Current update level=0)			

In both cases, the user enters the lower and upper bounds *in linear space*. If linear-uniform is selected, a uniform distribution between the lower and upper bounds is assumed; if log-uniform is selected, a uniform distribution between the *log* of the lower and upper bounds is assumed. For example, if the lower and upper bounds were chosen as 10 and 1000, the median value would be 100 (10^{3-1}) if log-uniform was selected, and 505 ($(9990)/2$) if linear-uniform was selected.

A-2.3 Triangular Distribution

The triangular distribution takes two forms: linear or log. Once a triangular distribution is selected, the user toggles between linear and log using the <F3> key. The linear and log input windows for the triangular distribution are identical (except for the field which identifies the window as linear or log):

In both cases, the user enters the lower bound, upper bound, and most likely value *in linear space*. If linear-uniform is selected, a triangular distribution using the lower bound, upper bound, and most likely value is assumed; if log-triangular is selected, a triangular distribution using the *log* of the lower bound, upper bound, and most likely value is assumed. For example, if the lower and upper bounds were chosen as 10 and 1000, and the most likely value was 100, the median value would be 100 if log-triangular was selected, and 332.5 if linear-triangular was selected.

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Parameter Editing			
Identifier : STORH		Parameter No. : 31 of 39	
Description: Parameter Type : Stochastic (0)			
Save Time	F1=Prev type		
Edit Param	Sampling Bias : No Bias	F2=Next type	
Affects	log	F3=Log/Linear	
Function	Lower bound: 1 (Constant)		
	Most likely: 5 (Constant)		
	Upper bound: 17 (Constant)		
F1=Prev Param	F2=Next Param	F3=Add Param	F4=Delete Param
F5=Find Param	F6=Print Summary	F7=Display Dist.	F8=Expected Value
F9=Strategy	F10=System update / Current update level 0		

A-2.4 Cumulative Distribution

The cumulative distribution is used to specify a cdf (cumulative distribution function) directly.

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Parameter Editing			
Identifier : STORH		Parameter No. : 31 of 39	
Description: Parameter Type : Stochastic (0)			
Save Time	F1=Prev type		
Edit Param	Sampling Bias : No Bias	F2=Next type	
Affects	log	F3=Log/Linear	
Function	Lower bound: 1 (Constant)		
	Most likely: 5 (Constant)		
	Upper bound: 17 (Constant)		
F1=Prev P	F2=Next P	F3=Add P	F4=Delete P
F5=Find P	F6=Print Summary	F7=Display Dist.	F8=Expected Value
F9=Strategy	F10=System update / Current update level 0		

The user specifies the cumulative distribution by entering value/cumulative probability pairs. A given pair (V,P) implies that the cumulative probability of V is equal to P. Note that, by definition, the first cumulative probability specified must be 0 and the last cumulative probability specified must be 1. Cumulative probabilities between the first and the last must be entered in ascending order (i.e., $P_{i+1} > P_i$). The user can type in up to 10 value/cumulative probability pairs. The values and cumulative probabilities *must be entered as numbers* and cannot be specified as parameters.

A-2.5 Discrete Distribution

The discrete distribution is used to specify a discrete pdf (probability density function) directly.

The user specifies the probability density function by entering value/probability density pairs. A given pair (V,P) implies that the probability of V is equal to P. Note that, by definition, the sum of the probabilities must be 1. The user can type in up to 10 value/probability density pairs. The values and probability densities *must be entered as numbers* and cannot be specified as parameters.

Repository Integration Program (Rev. 4.04)

General PA Model Strategy Model Results

Parameter Editing

Identifier : STOCH1 Parameter No. : 31 of 39

Description:

Parameter Type : DISCRETE DISTRIBUTION

Sampling Bias: Bias

Save Time H

Edit Param

[Affects

#	Value	Probability
1	0	0
2	0	0
3	0	0
4	0	0
5	0	0
6	0	0
7	0	0
8	0	0
9	0	0
10	0	0

(Sum of P's must =1, exp. values in ().)

F1=Prev type
F2=Next type

F1=Prev Par
F5=Find Par
F9=Strategy

A-2.6 Poisson Distribution

The only input parameter for the Poisson distribution is the expected number of occurrences (the rate times the distance unit or the time unit).

Repository Integration Program (Rev. 4.04)

General PA Model Strategy Model Results

Parameter Editing

Identifier : STOCH1 Parameter No. : 31 of 39

Description:

Parameter Type : Stochastic

(0)

Save Time

Edit Param

[Affects

POISSON DISTRIBUTION

Sampling Bias : No Bias

Expected Value : 0 (Constant)

[Function of]-

F1=Prev Param F2=Next Param F3=Add Param F4=Delete Param
F5=Find Param F6=Print Summary F7=Display Dist. F8=Expected Value
F9=Strategy F10=Bayesian update (Current update level=0)

A-2.7 Beta Distribution

The Beta distribution requires a mean, a standard deviation, a minimum value, and a maximum value.

Repository Integration Program (Rev. 4.04)

General PA Model Strategy Model Results

Parameter Editing

Identifier : STOCH1 Parameter No. : 31 of 39

Description:

Parameter Type : Stochastic

(0)

Save Time

Edit Param

Affects

Function

F1=Prev Pa

F5=Find Pa

F9=Strategy

BETA DISTRIBUTION

Sampling Bias : No Bias

MEAN : 0 (Constant)

S.D. : 0 (Constant)

MIN : 0 (Constant)

MAX : 0 (Constant)

(Equivalent # successes: 0)

(# failures : 0)

F1=Prev type

F2=Next type

F1 Bayesian update (Current update level=0)

The upper and lower bounds simply define a translation and scaling of the underlying distribution, and the mean and standard deviation are converted internally to the two arguments of the "classical" beta distribution, I and 9 (see Section A-1.10). There is a direct relationship between I and 9 and the results of a binomial trial: I corresponds to the "number of successes - 1" and 9 corresponds to the "number of failures - 1". At the bottom of the binomial window, the corresponding number of successes and number of failures are calculated and displayed based on the scaled mean and standard deviation entered by the user.

A-2.8 Gamma Distribution

The Gamma distribution requires a mean and a standard deviation.

Repository Integration Program (Rev. 4.04)

General PA Model Strategy Model Results

Parameter Editing

Identifier : STOCH1 Parameter No. : 31 of 39

Description:

Parameter Type : Stochastic

(0)

Save Time

Edit Param

Affects

Function

F1=Prev Pa

F5=Find Pa

F9=Strategy

Gamma Distribution

Sampling Bias : No Bias

Mean : 0 (Constant)

S.D. : 0 (Constant)

F1=Prev type

F2=Next type

F3=Truncated

F1 Bayesian update (Current update level=0)

F2 Bayesian update (Current update level=0)

F3 Bayesian update (Current update level=0)

F4 Bayesian update (Current update level=0)

F5 Bayesian update (Current update level=0)

F6 Bayesian update (Current update level=0)

F7 Bayesian update (Current update level=0)

F8 Bayesian update (Current update level=0)

F9 Bayesian update (Current update level=0)

The <F5> key can be used to specify minimum and maximum bounds.

A-2.9 Weibull Distribution

The Weibull distribution requires three parameters: the minimum value (M), the Weibull slope or shape factor (I), and the difference between the Weibull scaling factor (9) and the minimum value (9-M). This last parameter is approximately equal to the mean value - the minimum value.

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Parameter Editing			
Identifier : STOCH1		Parameter No. : 31 of 39	
Description:			
Parameter Type : Stochastic			
(0)			
Save Time	WEIBULL DISTRIBUTION		
Edit Param	Sampling Bias : No Bias	F1=Prev type	
[Affects		F2=Next type	
		F5=Truncated	
[Function	Min. (ε) : 0	(Constant)	
	Weibull slope (α) : 0	(Constant)	
	Mean-Min (b-ε) : 0	(Constant)	
F1=Prev Param	F2=Next Param	F3=Add Param	F4=Delete Param
F5=Find Param	F6=Print Summary	F7=Display Dist.	F8=Expected Value
F9=Strategy	F10=Bayesian update (Current update level=0)		

The <F5> key can be used to specify minimum and maximum bounds.

A-2.10 Binomial Distribution

The Binomial distribution requires a batch size (i.e., the number of picks), and a probability of occurrence.

Repository Integration Program (Rev. 4.04)			
General	PA Model	Strategy Model	Results
Parameter Editing			
Identifier : STOCH1		Parameter No. : 31 of 39	
Description:			
Parameter Type : Stochastic			
(0)			
Save Time	BINOMIAL DISTRIBUTION		
Edit Param	Sampling Bias : No Bias	F1=Prev type	
[Affects		F2=Next type	
[Function	No. Picks : 0	(Constant)	
	Probability: 0	(Constant)	
F1=Prev Param	F2=Next Param	F3=Add Param	F4=Delete Param
F5=Find Param	F6=Print Summary	F7=Display Dist.	F8=Expected Value
F9=Strategy	F10=Bayesian update (Current update level=0)		

A-2.11 Boolean Distribution

The Boolean distribution requires a single input: the probability of being true. The parameter takes on one of two values: 0 if false, and 1 if true.

Repository Integration Program (Rev. 4.04)															
General	PA Model	Strategy Model	Results												
Parameter Editing		Parameter No. : 31 of 39													
Identifier : STOCH1															
Description:															
Parameter Type : Stochastic															
(0)															
<table border="1"> <thead> <tr> <th colspan="2">BOOLEAN DISTRIBUTION</th> </tr> </thead> <tbody> <tr> <td>Save Time</td> <td>F1=Prev type</td> </tr> <tr> <td>Edit Param</td> <td>F2=Next type</td> </tr> <tr> <td>[Affects</td> <td></td> </tr> <tr> <td colspan="2">Sampling Bias : No Bias</td> </tr> <tr> <td colspan="2">Probability of true : 0 (Constant)</td> </tr> </tbody> </table>				BOOLEAN DISTRIBUTION		Save Time	F1=Prev type	Edit Param	F2=Next type	[Affects		Sampling Bias : No Bias		Probability of true : 0 (Constant)	
BOOLEAN DISTRIBUTION															
Save Time	F1=Prev type														
Edit Param	F2=Next type														
[Affects															
Sampling Bias : No Bias															
Probability of true : 0 (Constant)															
[Function of]-															
F1 Prev Param	F2 Next Param	F3 Add Param	F4 Delete Param												
F5 Find Param	F6 Print Summary	F7 Display Dist.	F8 Expected Value												
F9 Strategy	F10 Bayesian update (Current update level 1)														

APPENDIX B

SPECIFYING STOCHASTIC FRACTIONS

At several locations within the user interface, the required input involves specifying how something is partitioned between several options. For example, if more than one water contact mode is defined, the user must specify how the waste packages are distributed between the modes. Similarly, when defining discharge pathways, the user must specify how mass is to be distributed between the defined pathways. By definition, the various fractions distributed to each option must sum to one.

If these fractions were known with certainty, they could be specified directly as actual fractions which sum to one. If these fractions were uncertain, however, they would have to be specified stochastically (as probability distributions), in which case they would not necessarily sum to one. One solution would be to sample the distributions of the various fractions each realization and then normalize each fraction such that the total does sum to one. This alternative, however, has the effect of "warping" the specified distributions. That is, the distributions which were specified by the user would not actually be the distributions that were realized (due to the post-processing normalization step).

RIP therefore utilizes a different approach to representing these kinds of inputs. Instead of inputting *actual fractions* (which must sum to one), the user inputs the *fraction of the remaining balance*. In this approach, the order in which the options are specified is important.

This approach is best illustrated by a simple example (using water contact modes). Consider three water contact modes: A, B, and C. Assume that the waste packages are distributed between these modes as follows: A (0.40), B (0.50), and C(0.10). The equivalent representation of this data in terms of fraction of the remaining balance is A(0.40), B(0.833), and C(1.0). That is, 0.40 of the waste packages are first assigned to contact mode A, 0.833 of the balance (which is 0.6 in terms of the actual fraction) is then assigned to contact mode B (since $0.833 \times 0.6 = 0.5$), and all (1.0) of the balance (which is 0.10 in terms of the actual fraction) is assigned to contact mode C.

This can be represented mathematically as follows:

Let

$X_i =$ the fraction of remaining balance for option i; and

$Y_i =$ the actual fraction for option i.

Then, given a set of actual fractions, ($Y_1 \dots Y_N$), these can be represented in terms of fraction of the remaining balance as follows:

$$X_i = \frac{Y_i}{B_i} \quad (B.1)$$

where:

$$Y_i = 1 - \sum_{j=1}^{i-1} (X_j)(B_j) \quad (B.2)$$

and by definition,

$$B_1 = 1 \text{ and } X_N = 1.$$

In these equations, B_i represents the remaining balance (in terms of an actual fraction) after distributing the $(i-1)$ th fraction.

The example presented above can be summarized below using the same nomenclature:

water contact mode	actual fraction (Y_i)	remaining balance (B_i)	fraction of remaining balance* (X_i)
A	0.4	1	0.4
B	0.5	0.6	0.8333
C	0.1	0.1	1.0

* This is what must actually be input into RIP.

As can be seen, specifying the fractions stochastically poses no difficulty, as long as we require that the final option be assigned a fraction of the remaining balance equal to one (and the user interface ensures that this is indeed the case). In effect, after realizing the fraction of the remaining balance stochastically for each but the last option, we are assigning whatever remains to the final option.

Given this approach, it should be apparent that the order in which the fraction of remaining balances are specified is important when the fraction need to be represented stochastically. The user should follow two rules (listed here in order of priority) when specifying the correct order for the fractions:

- 1) Fractions should be specified with the smallest first and the largest last. This is particularly important when there are large differences (e.g., 0.001 as compared to 0.5) between the various options. The last option should be reserved for the "most likely option" (i.e., the "nominal" or "base case"), whose actual fraction depends on the distributions to the other options.
- 2) Fractions with a low degree of uncertainty should be specified before similar-sized fractions whose uncertainty is greater.

APPENDIX C

NORMALIZATION OF RESULTS

As discussed in the text, several of the outputs generated by RIP are currently normalized to U.S. regulatory limits. In particular, the *Waste Package Release Rate* is normalized to 10 CFR 60.113 and the *Cumulative Release to AE* is normalized to 40 CFR 191.13. When selected, these two results are always normalized. The remaining RIP outputs (with the exception of time histories and concentration\dose\risk results) represent cumulative releases (e.g., from specific waste package groups or pathways). The user has the choice of normalizing these results (according to 40 CFR 191.13) or displaying them directly (in units of Curies). Time histories are never normalized and are always presented in units of Curies.

The normalization procedures used by the software are described below. Note that all calculations carried out within RIP are in units of mass (grams), which are converted to Curies when appropriate by multiplying by the specific activity.

40 CFR Part 191.13

This regulation requires that cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal shall have a likelihood of less than 0.1 of exceeding specified release limits and less than 0.01 of exceeding ten times the specified release limits. RIP normalizes releases to these specified limits to facilitate evaluation of this regulation.

The normalized result, N_i , for radionuclide i is computed as follows:

$$N_i = \frac{R_i}{\text{NORM}_i} \quad (\text{C.1})$$

where:

N_i = normalized cumulative release for radionuclide i (unitless);

R_i = cumulative release for radionuclide i (grams);

NORM_i = normalization factor for radionuclide i (grams);

and

$$\text{NORM}_i = \frac{\text{LIMFAC} \times \text{RL}_i}{a_i} \quad (\text{C.2})$$

where:

LIMFAC = total *effective* metric tons of heavy metal in repository (MTHM);

RL_i = regulatory release limit for radionuclide i (Ci/MTHM);

a_i = specific activity for radionuclide i (Ci/g).

LIMFAC is defined as follows:

$$\text{LIMFAC} = \sum_{j=1}^{\text{WPT}} (M_j \times \text{NWP}_j \times f_b) \quad (\text{C.3})$$

where:

- M_j = the equivalent metric tons of heavy metal for waste package type j ;
- f_b = a factor which modifies the equivalent metric tons of heavy metal according to $BURNUP_j$, the equivalent waste burnup (in MWd/MTHM) for waste package type j ;
- WPT = the number of waste package types; and
- NWP_j = number of waste packages of type j ;

f_b is computed as follows:

- 1) if $25,000 < BURNUP_j < 40,000$, $f_b = 1$;
- 2) if $BURNUP_j \geq 40,000$,

$$f_b = \frac{\min(BURNUP_j, 100,000)}{30,000} \quad (C.4)$$

- 3) if $BURNUP_j \leq 25,000$,

$$f_b = \frac{\max(BURNUP_j, 5000)}{30,000} \quad (C.5)$$

The total normalized release from the repository is calculated by summing the contributions from all radionuclides:

$$N = \sum_{i=1}^{NRN} N_i \quad (C.6)$$

where

- N = total normalized cumulative release (unitless); and
- NRN = number of radionuclides.

Note that radionuclides which have been specified as having a regulatory limit of zero are skipped in this summation (i.e., N_i is set to zero).

The regulatory release limits are given here in terms of MTHM. For high-level wastes generated from reprocessing, the equivalent MTHM and the burnup should be in terms of the fuel from which the reprocessed waste was generated. The regulations specify other units for the release limits (i.e., other than MTHM) which are appropriate under some circumstances. This is not currently accommodated in RIP. That is, waste packages must be specified in terms of an equivalent MTHM and burnup.

10 CFR Part 60.113

This regulation requires that the release rate of any radionuclide from the engineered barrier system following the containment period shall not exceed 10^{-5} of the inventory of that nuclide calculated to be present at 1000 years following permanent closure. This requirement does not apply to any radionuclide which is released at a rate less than 10^{-3} (0.1%) of the calculated total release limit. The total release limit (per year) is equal to 10^{-5} of the total inventory of all radionuclides (e.g., in Curies) at 1000 years. RIP normalizes annual releases for each radionuclide to 10^{-5} of the 1000 year inventory for that radionuclide, and saves the maximum normalized annual release (and the corresponding radionuclide responsible for that release) every realization. RIP assumes a containment period equal to 1000 years (i.e., only releases after 1000 years are considered).

The steps for computing this maximum annual normalized release are as follows:

- 1) Compute the total inventory, TI_i , for each radionuclide i in the repository at the time of closure:

$$TI_i = \sum_{j=1}^{WPT} (NWP_j \times MW_j \times I_{ij}) \quad (C.7)$$

where:

TI_i = total inventory for radionuclide i in repository at time of closure (grams);

I_{ij} = the inventory of radionuclide i in waste package type j at time of closure (grams/gram waste matrix);

WPT = number of waste package types;

NWP_j = number of waste packages of type j ; and

MW_j = total mass of waste matrix for waste package type j .

Note that the initial inventory for each individual radionuclide in each waste package (I_{ij}) must be input by the user as the inventory at the *time of closure* (at which time the waste may actually have an age of 50 to 100 years, depending on the disposal and closure schedule).

- 2) Carry out decay calculations and compute TI_i^* , the inventory for each radionuclide i in the repository at 1000 years after closure.
- 3) Compute the total annual release rate limit:

$$TRL = \sum_{i=1}^{NRN} 10^{-5} \times TI_i^* \times a_i \quad (C.8)$$

where:

TRL = total annual release rate limit (Ci/yr);

NRN = the number of radionuclides; and

a_i = specific activity for radionuclide i (Ci/g).

4) Every time step, loop through all the radionuclides as follows:

a) compute the annual release rate as follows:

$$ran_i = \frac{r_i}{\Delta t} \quad (C.9)$$

where:

ran_i = annual waste package release rate (summed over all groups) for current timestep for radionuclide i (g/yr);

r_i = waste package release (summed over all groups) for current timestep for radionuclide i (g); and

Δt = length of timestep (yrs).

b) check to see if release is significant (high enough to be regulated); if it is, normalize release to 10^{-5} of the 1000 yr inventory for the radionuclide, and test to see if this is the maximum release (for any radionuclide) so far for this realization:

```

if ( $ran_i \times a_i > TRL \times 10^{-3}$ ) then
    norm =  $ran_i \div (TI_i \times 10^{-5})$ 
    maxnorm = MAXIMUM of maxnorm and norm
end if
    
```

5) This procedure results in a single value for each realization: the maximum normalized annual release from a waste package for any radionuclide. The ID of the radionuclide is also saved. RIP also saves the fraction of waste packages failed at 300 years and 1000 years for each realization to help evaluate "substantially complete containment".

APPENDIX D
ERROR REPORTING

Two forms are included in this appendix for error reporting. The first, "RIP Software Problem Report", is to be used for reporting errors or problems with the software. The second, "RIP Software Change Request", is to be used to suggest changes or modifications to the software.

When forwarding a RIP Software Problem Report, it is most effective to include on a disk the associated .rp input file.

Forms (and disks) should be forwarded to:

Rick Kossik
Golder Associates Inc.
4104 148th Ave NE
Redmond, Washington 98052
(206) 883-0777
(206) 882-5498 (fax)
rkossik@golder.com (e-mail)

RIP Software Problem Report

Front End Version:	Back End Version:
Problem Description (use additional pages as needed):	
.rp file name (if enclosed):	
Submitted by:	Date:

Golder Analyst:
Golder Comments:

Description of Change:	
Reason for Request:	
Submitted by:	Date:

Golder Comments:

Golder Analyst:
Golder Comments:

APPENDIX E

IMPLEMENTING CODED FUNCTIONS

This appendix discusses the specific programming changes that must be made to the source code in order to add a coded function to RIP.

E-1 OVERVIEW

Coded functions are external calculations or other manipulations that are not included in the standard arithmetic of RIP. They currently include buffering algorithms for saving values, two complex special purpose models, and simple test functions to test the coded function interface. The coded function facility allows special purpose calculations or manipulations to be accomplished with more flexibility, speed or complexity than with the standard RIP programmatic elements.

Implementing a coded function requires three separate elements:

1. The *front end* must contain information about each external coded function so that a user can reference it by name and assign the correct number of arguments. It must also include an integer reference for the *back end*.
2. A special function, *eval*, family, is responsible for transferring the information passed from main body of the RIP *back end* to the arguments of each coded function and for calling the function.
3. The coded function itself.

In the current version of RIP, no more than twenty coded functions can be defined. It should also be noted that removing or altering a coded function may cause some of the verification checks to fail.

E-2 THE CODED FUNCTION

The implementation of the coded function is left to the programmer, but several restrictions apply so that the functions can be correctly called by RIP. They are:

- The function must have no return value (e.g., void functions in C, or subroutines in FORTRAN).
- Data are passed from RIP to the coded function and back again to RIP via arguments.
- The function may not have more than 70 input arguments and 30 output arguments and must have at least one of each.
- Input arguments may not be modified by the coded function.
- Each argument must be single value, single precision, floating point type.

- Functions that have 'hidden' dependencies, such as a simulation function that requires one or more initialization functions, must have one *dependency* input argument for every dependency that is used only by RIP to schedule their execution.

Furthermore, in the current version of RIP, no more than twenty separate coded functions can be defined.

E-3 BACK-END MODIFICATIONS

After creating the function, the call to the function must be implemented. This is accomplished in the file `coded.c`. The file is written in C and contains a function, `eval_family`, that contains one call for each coded function. The call to the coded function is controlled by a `switch` statement:

```
switch (f->type){
    case 1: if (f->update)
        A_plus_B(inargs[0], inargs[1], &outargs[0]); break;
    case 2: if (f->update)
        A_minus_B(inargs[0], inargs[1], &outargs[0]); break;
    case 3: if (f->update)
        A_multiply_B(inargs[0], inargs[1], &outargs[0]); break;
    case 4: if (f->update)
        A_divide_B(inargs[0], inargs[1], &outargs[0]); break;
    .
    .
    .
    default: break;
}
```

A new `case` statement with an integer constant must be added to the `switch` block or an existing coded function must be replaced. The only valid integer constants for the `case` statements are the values from 1 to 20, inclusive. Furthermore, each constant must be unique because the value of the constant corresponds to a unique position in three control arrays that are used to define the coded functions in the *front end*. For example, if the third `case` statement is used for a coded function in the *back end*, in the *front end* it must be the third element of the control arrays `codedtypesids`, `numcodedinputs`, and `numcodedoutputs` that must be modified.

Finally, the number of input and output arguments must match the function definition.

Below is an example of a simple coded function, which has been used as a test routine. It takes two input and one output arguments. The output is the sum of the two inputs.

```
static void A_plus_B( float inarg1, float inarg2, float *outarg1)
{
    *outarg1 = inarg1 + inarg2;
}
```


E-4 FRONT-END MODIFICATIONS

The user must edit a special table that sets the coded function properties, Figure E-1. This table is stored in the RIP data file. There is no need to alter the RIP program. To edit the table select **General** in the RIP program and use the key F2.

Repository Integration Program (Rev. 4.03)							
General		PA Model		Strategy Model		Results	
Select Output							
Coded Function Definitions							
No.	Name	# Inputs	# Outputs	No.	Name	# Inputs	# Outputs
1	A+B=C	2	1	11	STINIT	21	1
2	A-B=C	2	1	12	TMSTEP	26	38
3	A*B=C	2	1	13	RADON	13	3
4	A/B=C	2	1	14	N/A	0	0
5	SAVE1	1	1	15	N/A	0	0
6	SAVE2	2	2	16	N/A	0	0
7	SAVE3	3	3	17	N/A	0	0
8	SAVE10	10	10	18	N/A	0	0
9	N/A	0	0	19	N/A	0	0
10	CMINIT	73	1	20	N/A	0	0

Figure E-1 — Table of Coded Function Definitions

The six character name is used to identify the coded function in the *front end*. The number of arguments must also be modified to insure that the user inputs the correct number of arguments. These values are used for a data check in the front-end and to transfer the required number of values to and from the coded functions in the back end. The position of the function description in the table is also critical. It must correspond to the integer constant in the *switch* block in the function `eval_family`. For example, the first function, 'A+B=C', will trigger a call to the line `case 1:` in `eval_family`.

Note that the table must contain the full complement of names and argument numbers for any possible coded functions in the *front end*, but that some may be place holders, 'N/A', or simple test routines, 'A/B=C'. The user must replace one of the existing entries in the table when adding a new coded function.

E-5 TESTING THE CODED FUNCTIONS

The RIP *post processor* may be used to check the calculation of a coded function by checking the value of its output arguments. It is also recommended that any coded function also be tested in a stand-alone program independently of RIP. This avoids some of the complexity of RIP and provides simpler debugging and independent testing.

APPENDIX F

EXAMPLE ASCII OUTPUT FILE

This appendix presents an example of an ASCII output file, which can be created by hitting <F2> from the main post-processor menu..

```

Run description                               : User's Guide Tutorial
Parameter file name                           : TUTPOST.bpf
Model Name                                   : TUTPOST.RP
Front End Version                             : 402D
Parameter Unit Version                       : 100r
Parameter file(.BPF): Date                   : 09-01-95 Time: 15:56:52
Total number of parameters                   :      8
# of Stochastics                             :      5
# of Events                                  :      1
# of Functions                               :      2
# of Tables                                  :      0
# of Coded Functions                         :      0
Header Position in the .BPF File             : 234
Statistic File Name                           : TUTPOST.bsr
Statistic file (.BSr)                        : Date: 09-01-95 Time: 15:56:52
# of realizations                            : 10
# of Radionuclide Species                    : 55
AC227   AM241   AM242   AM242M   AM243   C14
CA41    CL36    CM243   CM244    CM245   CM246
CO60    CS135   CS137    H3      I129    MO93
NB-S1    NB93    NB94    NI-S1    NI59    NI63
NP236    NP237   PA231    PB210    PD107    PU238
PU239    PU240   PU241    PU242    RA226    RA228
SE-S1    SE79    SM151    SN-S1    SN126    SR90
TC99     TH228   TH229    TH230    TH232    U232
U233     U234    U235     U236     U238     ZR-S1
ZR90
# of Categories in Statistics                 : 4
# of Statistic results                       : 115
Header Position in Statistic File            : 802
Time History File Name                       : TUTPOST.btr
Time History File Date                       : 09-01-95 Time : 15:56:52
Data block data position                     : 51807
# of Categories in Time History              : 4
# of Time History Results                    : 115
# of Time Histories                         : 5
Header Position in Time History File         : 1031
Total Simulation Time                        : 1000
Time Step                                    : 100
.....
Parameter Data
.....
Parameter ID   Realization   Value      Probability
A1             1             3.29503E+00  0.2550
A1             2             1.08009E+00  0.0089
A1             3             6.83754E+00  0.6486
A1             4             3.94773E+00  0.3275
A1             5             1.17543E+00  0.0195
A1             6             1.25443E+00  0.6949
A1             7             1.40285E+00  0.0448
A1             8             4.37826E+00  0.3754
A1             9             8.02646E+00  0.7807
A1            10             1.39677E+00  0.0441
FLOW           1             2.95500E+02  0.6085
FLOW           2             2.75493E+02  0.2340
FLOW           3             2.77358E+02  0.2636
FLOW           4             2.95217E+02  0.6030
FLOW           5             3.18719E+02  0.9245
FLOW           6             2.74742E+02  0.2227
FLOW           7             2.78206E+02  0.2776
FLOW           8             2.69994E+02  0.1586
FLOW           9             3.06012E+02  0.7884
FLOW          10             2.77718E+02  0.2695
KD             1             1.00000E+00  0.0000
KD             2             1.00000E+00  0.0000
KD             3             1.00000E+00  0.0000
KD             4             1.00000E+00  0.0000

```

KD	5	1.00000E+00	0.0000
KD	6	1.00000E+00	0.0000
KD	7	1.00000E+00	0.0000
KD	8	1.00000E+00	0.0000
KD	9	1.00000E+00	0.0000
KD	10	1.00000E+00	0.0000
OMEGA	1	9.91216E-04	0.4913
OMEGA	2	4.10901E-04	0.0142
OMEGA	3	1.32370E-03	0.7555
OMEGA	4	1.45718E-03	0.8235
OMEGA	5	1.51822E-03	0.8484
OMEGA	6	5.02602E-04	0.0449
OMEGA	7	1.56063E-03	0.8638
OMEGA	8	1.37729E-03	0.7852
OMEGA	9	2.80410E-03	0.9945
OMEGA	10	1.16859E-03	0.6498
PI	1	3.14170E+00	0.0000
PI	2	3.14170E+00	0.0000
PI	3	3.14170E+00	0.0000
PI	4	3.14170E+00	0.0000
PI	5	3.14170E+00	0.0000
PI	6	3.14170E+00	0.0000
PI	7	3.14170E+00	0.0000
PI	8	3.14170E+00	0.0000
PI	9	3.14170E+00	0.0000
PI	10	3.14170E+00	0.0000
EVENT	1	1.00000E+00	0.0000
EVENT	2	1.00000E+00	0.0000
EVENT	3	1.00000E+00	0.0000
EVENT	4	1.00000E+00	0.0000
EVENT	5	1.00000E+00	0.0000
EVENT	6	1.00000E+00	0.0000
EVENT	7	1.00000E+00	0.0000
EVENT	8	1.00000E+00	0.0000
EVENT	9	1.00000E+00	0.0000
EVENT	10	1.00000E+00	0.0000
AREA	1	1.03520E+01	0.0000
AREA	2	3.39333E+00	0.0000
AREA	3	2.14815E+01	0.0000
AREA	4	1.24026E+01	0.0000
AREA	5	3.69223E+00	0.0000
AREA	6	2.27912E+01	0.0000
AREA	7	4.40734E+00	0.0000
AREA	8	1.37552E+01	0.0000
AREA	9	1.52167E+01	0.0000
AREA	10	1.38822E+00	0.0000
TMFFUN	1	2.00000E+02	0.0000
TMFFUN	2	2.00000E+02	0.0000
TMFFUN	3	2.00000E+02	0.0000
TMFFUN	4	2.00000E+02	0.0000
TMFFUN	5	2.00000E+02	0.0000
TMFFUN	6	2.00000E+02	0.0000
TMFFUN	7	2.00000E+02	0.0000
TMFFUN	8	2.00000E+02	0.0000
TMFFUN	9	2.00000E+02	0.0000
TMFFUN	10	2.00000E+02	0.0000

Statistics Data

Category Description : Cumulative Release from All WPs
Release from All WPs

Category	Value
1	8.16948E+06
2	2.57860E+06
3	1.64841E+07
4	1.04032E+07
5	3.44409E+06
6	1.72507E+07
7	3.39698E+06
8	1.01501E+07
9	2.22403E+07
10	3.37368E+06

Category Description : Cum. Release from WP or Pathways to AE