Performance Assessment Uncertainty Analysis for Japan's HLW Program Feasibility Study (H12)

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ABSTRACT

Most HLW programs in the world recognize that any estimate of long-term radiological performance must be couched in terms of the uncertainties derived from natural variation, changes through time and lack of knowledge about the essential processes. The Japan Nuclear Cycle Development Institute followed a relatively standard procedure to address two major categories of uncertainty. First, a Features, Events and Processes (FEPs) listing, screening and grouping activity was pursued in order to define the range of uncertainty in system processes as well as possible variations in engineering design. A "reference" and many "alternative" cases representing various groups of FEPs were defined and individual numerical simulations performed for each to quantify the range of conceptual uncertainty. Second, parameter distributions were developed for the reference case to represent the uncertainty in the strength of these processes, the sequencing of activities and geometric variations. Both point estimates using high and low values for individual parameters as well as a probabilistic analysis were performed to estimate parameter uncertainty. A brief description of the conceptual model uncertainty analysis will be presented. This paper focuses on presenting the details of the probabilistic parameter uncertainty assessment.

INTRODUCTION

The Japanese High Level Waste (HLW) program is nearing completion of its second feasibility analysis (The H12 Report) to be submitted to the Atomic Energy Commission of Japan toward the end of 1999. This report will provide a foundation for future site selection, regulation development, future R&D as well as establishing the process of performance assessment.

The research and development program at the Japan Nuclear Cycle Development Institute or JNC (successor of the Power Reactor and Nuclear Fuel Development Corporation) has, in general, followed a common international pattern (1) in which they list FEPs, develop scenarios and evaluate ranges of parameter uncertainty.

Scenarios were divided into two major categories based on qualitative judgement that certain large-scale disruptions would make it impossible to project future operating conditions. It is assumed that the FEPs associated with these large disruptions can be eliminated based on careful site selection. The remaining FEPs are divided into a series of cases. One of these, the "base case" represents an undisturbed, natural system with saturated groundwater flow from the repository to the biosphere defined as the primary radionuclide transport pathway. For the feasibility study defined in the current draft of the year 2000 feasibility report, JNC has defined a deterministic hypothetical site with fresh, high pH water in granitic rock with horizontally emplaced waste packages as the base system. This system forms the basis of the following uncertainty assessment. Alternative systems based on differences in rock type; water chemistry and geographic location are also considered but will not be discussed here.

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Parameter uncertainty was initially considered by making a series of deterministic model realizations in which one or more parameters were modified to either their reasonable maximum or reasonable minimum values. The results of these point specific calculations are reported in the current feasibility study. To augment this point wise analysis, a Monte Carlo calculation was performed using parameter distributions for a subset of parameters viewed as relatively important for the overall system.

BASE CASE SCENARIO

The reference scenario represents the expected behavior of a robust engineered barrier system (EBS) consisting of a vitrified-glass waste source within a steel overpack surrounded by a thick bentonite buffer within a fresh-water, moderately high-pH environment. This engineered barrier is emplaced in horizontal drifts within granite or a low-permeability sedimentary rock. The geologic pathway is conservatively estimated to be 100 meters from the edge of the repository, at which point migrating groundwater encounters a vertical migration path (fault) and is immediately transported to a groundwater aquifer. Finally, radionuclides exit the geosphere through a discharge connection from groundwater to surface water. A reference biosphere with a representative Japanese exposure group (farmers) was then developed in order to assess exposure and dose rates.
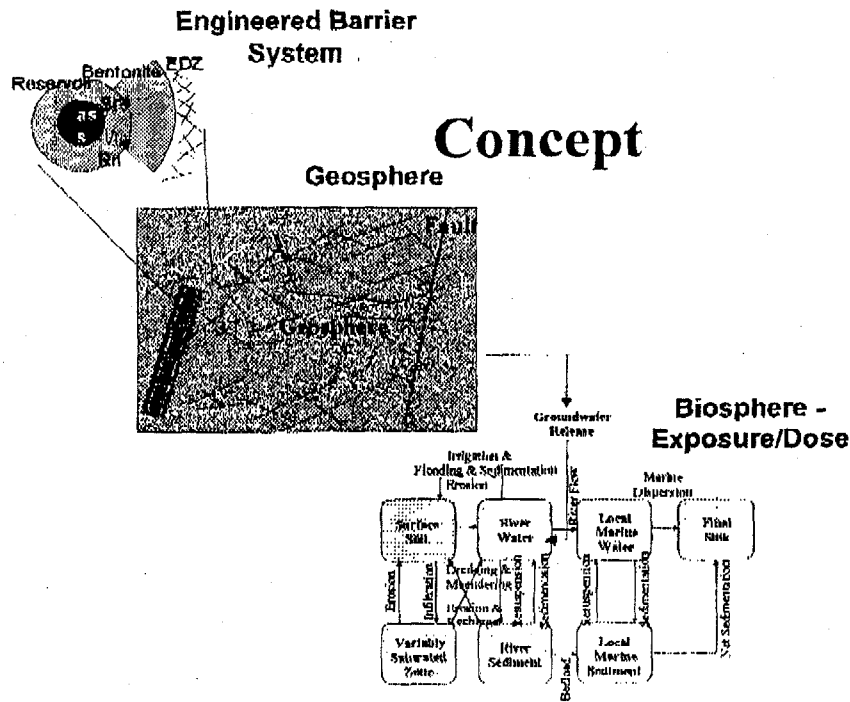

Figure 1. Schematic image of the reference case as represented by the three main modeling components.

PRIMARY MODEL CHAIN

The model chain used to represent the base case consists of four independent analysis tools: MESHNOTE for the engineered barrier system (EBS), PAWorks and MATRICS for the geosphere and AMBER for the biosphere.

Engineered Barrier System

MESHNOTE (2) is a finite element simulation code capable of representing the dissolution of glass with the corresponding release of radionuclides, radial migration of nuclides and silica away from the waste source along a 1D diffusion pathway through bentonite. MESHNOTE also accommodates radioactive decay along decay chains at all steps in the simulation process along with sorption to the bentonite clay and precipitation / dissolution along the transport path. This portion of the system is often referred to as the Engineered Barrier System (EBS). To a large degree, the release from the EBS is controlled by the outer concentration boundary condition. If one assumes that the concentration at this outer boundary is zero due to rapid advective migration away from the EBS within the geosphere then diffusion rates are relatively high. If however, advection near the EBS boundary is slower and thus the concentration near the boundary is greater than zero, this decrease in the concentration gradient produces a noticeable decrease in the total nuclide release from the EBS. The release from the EBS is introduced as a source term to the geosphere model.

Geosphere System

The PAWorks simulation code represents flow and transport through the geosphere as a connection of discrete pathways that correspond to a discrete fracture network concept. The model initially simulates discrete fractures then translates these fractures to a complex network of interconnected pipes. Flow then transport are solved within this pipe network. Because the fracture network is not deterministically defined, a series of 50 stochastic realizations were simulated to capture the numerical variation within the simulation process. The combined result for radionuclide flux release from the geosphere is connected to the biosphere model.

This approach using PAWorks can also be adequately represented by a combination of parallel-plate models, each of which represents a different portion of the distribution of transmissivity within fractures. This second approach was implemented using a parallel plate transport model called CRYSTAL (3, 4). The results of this parallel plate modeling approach is viewed as representative of the release from the entire repository in that the distribution of transmissivity can represent the spatial distribution of average transmissivities along the many transport paths.

Biosphere

The biosphere model (5) includes seven compartments and 15 transfer mechanisms between compartments as well as conversions from concentration to dose for several media representing the health effects consequent to specified exposure. The compartments represent volumes of water or geologic material primarily at the earth's surface. Transfer mechanisms represent the physical transfer of media such as water or solid particles (soil, sediment) between compartments. Exposure routes include ingestion, uptake by plants and animals as well as direct exposure. While three different sets of exposure pathways and receptors were originally considered, the highest exposure values were received by a "Farmer" receptor so we focus on doses to the farmer in this presentation. This conceptualization was implemented within a compartment model called AMBER (6, 7), which is very flexible in allowing the use to specify any number or type of compartments and transfer functions.

The model was run assuming unit input from each of the radionuclide species including a few short lives species that are not explicitly tracked in the previous EBS and geosphere models. The ratio of final dose to initial unit radionuclide input is used as a conversion factor for translating the results of the PAWorks or CRYSTAL release to an equivalent expression of human dose.

The full conceptual model is best observed in Figure 1.

CAPASA

To facilitate the quality assurance and easy of transfer between these three main codes, a systems framework called CAPASA was developed and implemented. It links the output of one code to the input of another, allows space for documentation and connects the output to graphics capabilities through a relatively easy to use graphics user interface. This framework is particularly important for tracking individual model runs and keeping track of input and their corresponding results.

Results are usually expressed as a time series of yearly dose to an individual from each radionuclide species and the time series of total yearly dose as a combination of all species.

PROBABILISTIC MODELING APPROACH

In order to rapidly evaluate the parameter uncertainty and provide a mechanism to evaluate certain of the alternative scenarios, an integrated model was developed within the code, RIP (8, 9). The objective of this second effort was to 1) provide an accuracy check on the primary model string by implementing a duplicate analysis and 2) use a code explicitly designed to implement and evaluate parameter uncertainty (10).

First, RIP models were developed and benchmarked against each of the three main component models of the original model chain. Then the three were linked to a single total system performance assessment (TSPA) model. During RIP development, the original model chain was also being modified so this process was repeated several times with various versions of the base case scenario.

Probabilistic Code Description

RIP combines a basic structure of mixing cells, pipes and various 1D pathways using advective or diffusive connections with a model to explicitly represent various source release mechanisms along with containers and other near-field engineered structures. This basic framework is complimented by a spreadsheet-like parameter and function definition model for building user specified process descriptions that can be linked with parameter definitions. Finally the code can be coupled to completely external codes or functions to represent highly complex processes.

RIP Model Development

The RIP base case model was developed to closely match the base case scenario described above. The simulation begins 1000 years after waste emplacement when it is assumed that the canisters fail. There are three major components of the model: the Engineered Barrier System (EBS), the geosphere and the biosphere.

The EBS consists of a glass waste source that degrades releasing both silica and radionuclides into a small surrounding reservoir of water. This reservoir surrounds the glass and is assumed to occupy the pore space generated through canister degradation. Surrounding the reservoir is a bentonite buffer divided into seven cylindrical shells. Finally, a cylindrical engineered disturbed zone cell (EDZ) surrounds the buffer. The geometry parameters for these cells including volume, masse, surface area and so forth are defined by the cylindrical geometry of the assumed waste emplacement. Once these assumed values are calculated, the geometry becomes irrelevant within RIP, which treats all these as a series of connected cells with diffusion connections.

The rate of radionuclide release is directly related to the rate of glass dissolution. For simulations with short time steps this was explicitly represented as an equation within RIP. For longer time

simulations – the small reservoir cycles between being saturated and unsaturated, thus an alternative approach was implemented. In the long-time frame approach, the rate of silica diffusion from the reservoir (which is often at its saturation level) into the first cell in the buffer was used as a surrogate for the rate of silica dissolution from the glass. This approach produces a slightly lower dissolution rate than the more accurate first approach. The results of this assumption and surrogate dissolution are obvious in a reduction in total release and dose estimates from Cs and a couple of other nuclides.

The source consists of 45 elements in three chains along with a set of independent nuclides. The transport of all nuclides is simulated simultaneously sharing solubility within nuclides of the same element. Diffusion through the 7 buffer cells is modulated by sorption on the bentonite matrix, the diffusion rate of the high porosity / low permeability media and the concentration gradient, which is primarily controlled by the external concentration boundary condition of the EDZ cell.

The Geosphere in RIP is represented by a set of 48 parallel 1D paths. These paths are combined into a single simulation pathway called a "Network Path" within RIP. All paths have certain common characteristics including diffusion depths, percentage of path area that is available for diffusion, mechanical dispersion in the longitudinal direction and so forth. However, paths vary in transmissivity, aperture, cross-section area and velocity. The diffusion rates and sorption parameters are consistent for all paths.

The release from the geosphere to the biosphere is assumed to consist of transport along a large subsurface conduit, possibly a fracture zone, to a shallow, high transmissivity aquifer. The aquifer discharges to surface streams or rivers releasing radionuclides into the biosphere. The AMBER based model described above produced a series of dose conversion factors that translate Bq/y release to the biosphere into uSv/y dose to the farmer receptor. The RIP model was not implemented to explicitly simulate the series of cells and transfers within the biosphere. Instead a dose conversion factor was developed for RIP consistent with the AMBER values defined for unit release rates. RIP requires that the DCF have units of (uSv/y / g/m3) of release from the geosphere. This was accomplished using the following translation –

$$DCF_{RIP}(\frac{\mu Sv/y}{g/m^3}) = DCF_{AMBER}(\frac{\mu Sv/y}{Bq/y}) \times SpecificActivity(\frac{Bq}{g}) \times Disch\arg eRate(m^3) \times 1000(\frac{\mu Sv}{mSv})$$

(eq 1.)

These DCF$_{RIP}$ values were then applied to the nuclide flux release from the geosphere measured in g/m^3.

Model Benchmarking

A standard approach to benchmarking was followed in which both simulation algorithms and results were compared (11). The EBS models developed using MESHNOTE and RIP produced results with very minor variation. Part of this variation can be ascribed to a difference between the two codes. RIP uses a fixed time step whereas MESHNOTE has a dynamically defined time step, which is quite small at early times and increases exponentially at later times. With a small initial time step, RIP accurately represents the early time sequence implemented in MESHNOTE. However, for RIP to represent the full time history or total time simulated in MESHNOTE requires a large initial time step, which creates some inconsistencies. First, during the first 5,000 years, RIP estimates for Cs release (the highest release) from the EBS are significantly lower than the

MESHNOTE results. However, after 10,000 years this discrepancy becomes small and the peak release is very similar. Smaller, but similar differences exist for other of the less significant nuclides.

The geosphere model and the biosphere model are nearly identical to that in the MESHNOTE-MATRICS-AMBER sequence so no other significant numerical differences exist.

The results of the benchmarking exercise are shown below. The nine radionuclides with highest peak releases in time < 1,000,000 years are shown in these series of graphs. You will notice that this discrepancy in Cs release from the EBS propagates through the early time release in the geosphere and produces a 15-20% miss-match in peak dose for Cs. Since Cs is the main dose contributor for this time frame, this miss-match is important and it may be possible to correct in future simulations. Otherwise the original base case model string and the RIP model string produce remarkable similar results using the constructs described above. Based on this similarity, the RIP model was then used for an initial uncertainty assessment.
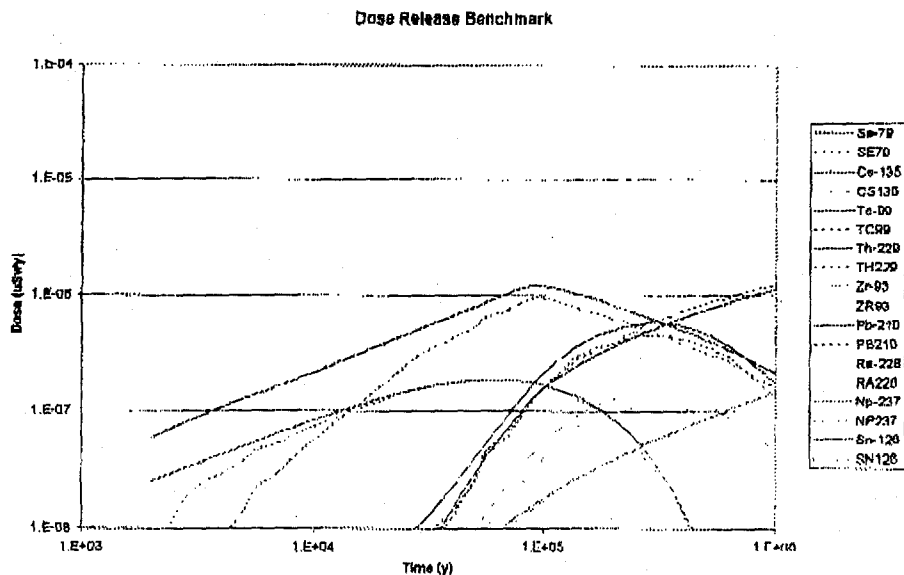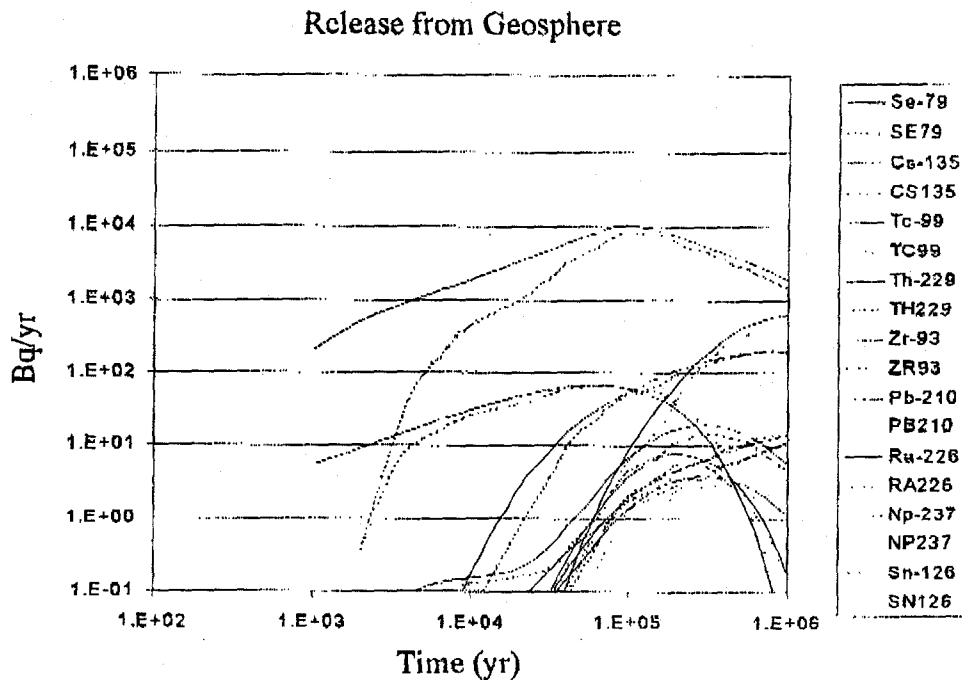
Release from the Biosphere

Release from Geosphere

Dose Release Benchmark
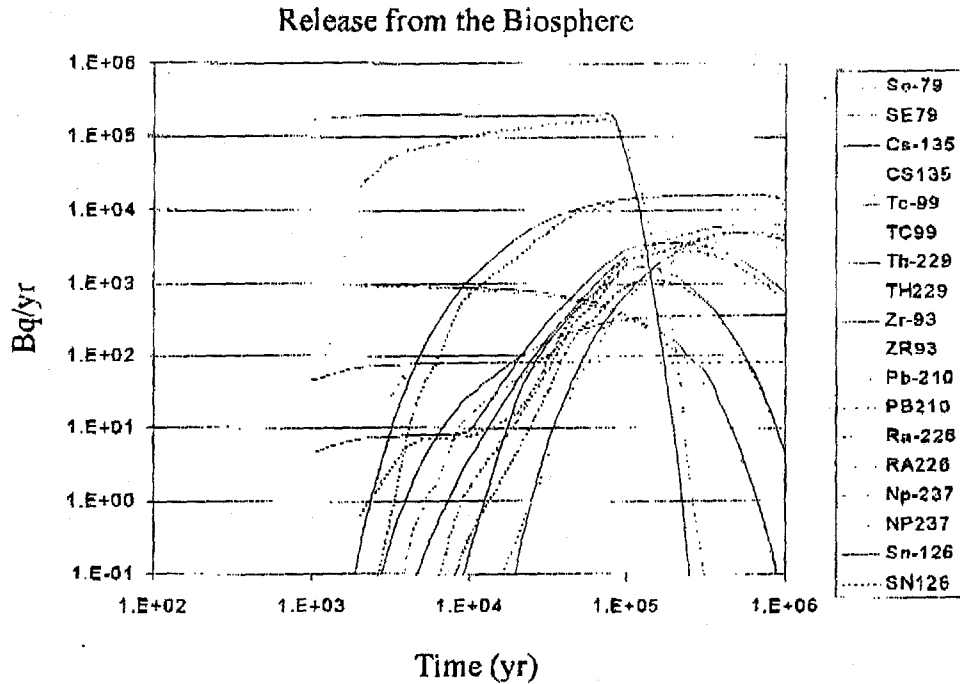
Figure 2. RIP Benchmarking Results for all Three Components of the modeling.

PROBABILITIC UNCERTAINTY ASSESSMENT

The linked RIP model was to perform a probabilistic uncertainty assessment based on Monte
Carlo approach in which the deterministic values for a subset of the full suite of parameters were
replaced by probability distributions. The parameters chosen for this initial uncertainty
calculation were selected as a function of preliminary point-wise sensitivity analysis performed
using the original model chain. The parameter values were defined based on reasonably wide
ranges based on existing data.

A second round of uncertainty assessment is planned in which most parameters will be evaluated based on a rigorous distribution definition process. Therefore, the current assessment can be viewed as a preliminary calculation used to establish the feasibility of the assessment, define a few of the uncertainty output types and gather some understanding of conceptual and model behavior.

Table 1 defines the parameters that were altered, the distribution functions used and the original base case values along with listing the RIP internal parameter name. All of these parameters were defined as part of the RIP spreadsheet type function then used as to define the cell and 1D pathway parameter inputs.

Table 1. Description of Uncertainty Parameter Values Used for the Uncertainty Assessment

Parameter	RIP Name	Uncertainty Description	Unit	Base Case Value
Engineered Barrier System				
Engineered Disturbed Zone Flux	QEDZ	U_L [0.001, 0.1]	m^3/y	0.01
Pore Diffusivity [2] in Bentonite	DpY	U [5.6e-10, 4.9e-9]	m^2/s	7.3e-10
Pore Diffusivity of Cs in Bentonite	DpCs	U [1.9e-10, 4.9e-10]	m^2/s	1.5e-9
Pore Diffusivity of Se in Bentonite	DpSe	U [1.7e-10, 1.95e-9]	m^2/s	4.9e-10
Retardation (Kd) Se	KbSe	U_L [0, 0.0005]	m^3/kg	0
Retardation (Kd) Zr	KbZr	U_L [1, 50]	m^3/kg	10
Retardation (Kd) Tc	KbTc	U_L [0.05, 10]	m^3/kg	1
Retardation (Kd) Sn	KbSn	U_L [1, 50]	m^3/kg	5
Retardation (Kd) Cs	KbCs	U_L [0.005, 0.05]	m^3/kg	0.01
Retardation (Kd) Sm	KbSm	U_L [0.5, 10]	m^3/kg	1
Retardation (Kd) Ra	KbRa	U_L [0.001, 0.01]	m^3/kg	0.01
Retardation (Kd) U	KbU	U_L [0.01, 50]	m^3/kg	1
Retardation (Kd) Np	KbNp	U_L [0.5, 10]	m^3/kg	1
Retardation (Kd) Am	KbAm	U_L [5, 100]	m^3/kg	10
Geosphere				
Porosity of the Rock	NG	U [0.01, 0.03]	-	0.02
Density of the Rock	DENR	2700 x (1-NG)	kg/m^3	2640
Effective Diffusivity	DEG	$(10^{-12.76}) \times NG^{2.0}$	m^2/s	3e-12
Dispersivity	DISP	U[1, 100]	m	10
Flow Wetted Surface of Fracture	FWS	U[0.10, 1.0]	%	0.5
Diffusion Depth	DIFDEP	U[0.03, 0.5]	m	0.1
Retardation (Kd) Se	KgSe	U_L [0, 0.1]	m^3/kg	0.01
Retardation (Kd) Zr	KgZr	U_L [0.01, 10]	m^3/kg	0.1
Retardation (Kd) Nb	KgNb	U_L [0.01, 10]	m^3/kg	0.1
Retardation (Kd) Tc	KgTc	U_L [0.05, 100]	m^3/kg	1
Retardation (Kd) Pd	KgPd	U_L [0.05, 1]	m^3/kg	0.1
Retardation (Kd) Sn	KgSn	U_L [0.1, 100]	m^3/kg	1
Retardation (Kd) Cs	KgCs	U_L [0.001, 10]	m^3/kg	0.05
Retardation (Kd) Sm	KgSm	U_L [0.05, 50]	m^3/kg	5

Retardation (Kd) Pb	KgPb	U_L [0.1, 10]	m^3/kg	0.1
Retardation (Kd) Ra	KgRa	U_L [0.05, 0.5]	m^3/kg	0.5
Retardation (Kd) Ac	KgAc	U_L [0.05, 50]	m^3/kg	5
Retardation (Kd) Th	KgTh	U_L [0.1, 10]	m^3/kg	1
Retardation (Kd) Pa	KgPa	U_L [0.1, 10]	m^3/kg	1
Retardation (Kd) U	KgU	U_L [0.1, 10]	m^3/kg	1
Retardation (Kd) Np	KgNp	U_L [0.1, 10]	m^3/kg	1
Retardation (Kd) Pu	KgPu	U_L [0.1, 10]	m^3/kg	1
Retardation (Kd) Am	KgAm	U_L [0.05, 50]	m^3/kg	5
Retardation (Kd) Cm	KgCm	U_L [0.05, 50]	m^3/kg	5

[1] – U_L – Log uniform distribution – uniform distribution in $\log_{10}$ space

[2] – Effective Diffusivity for all nuclides except Cs and Se

RESULTS

The uncertainty assessment shows that the average peak dose to receptor can vary by as much as half an order of magnitude within a single standard deviation or a total of 3 orders of magnitude over +/- 3 standard deviations. Figure 3 shows the mean dose (bold black line) for 100 realizations bracketed by +/- 1 standard deviation (bold blue and bold red lines). The amount of variance in the estimate appears to vary with time and increases between 10^4 and 10^6 years. Also shown are ten individual dose time series (thin black lines) these show that there are significant differences in the shape of the time series curve based on the uncertainty in the parameters selected. Thus, not only is the peak value significantly different, but also the time of the peak varies from about 5,000 years to 10^6 years depending on parameters chosen.
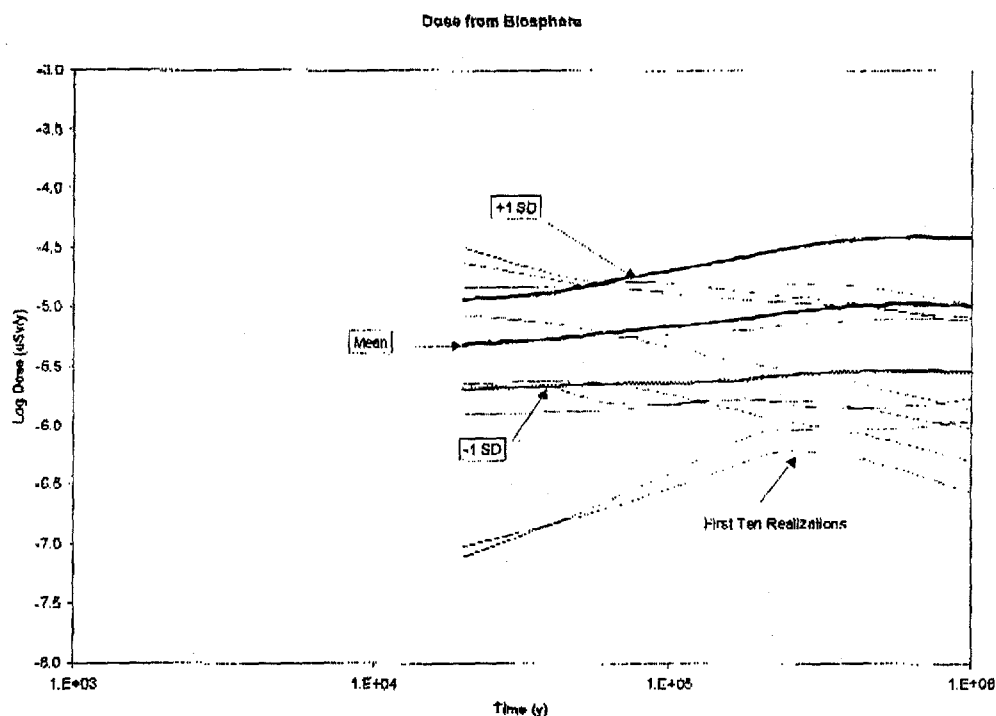

Dose from Biosphere

Figure 3. Time series of total dose from biosphere to receptor. Mean of 100 realizations along with +/- one standard deviation shown in bold lines. Also shown are the time series of total dose for first 10 realizations.

The two graphs in Figure 4 show the standard probability density function (PDF) and cumulative density functions (CDF) for the peak total dose to the farmer receptor. The maximum total dose estimated for the base case estimated by the original model string for the base case scenario was approximately 3.0E-6 µSv/y or −5.5 in log units. The RIP benchmark analysis produced a maximum estimate of approximately 2.0E-6 µSv/y or −5.7 log units. This second value is marked in the two graphs in Figure 4. This original estimate does not fall at the mean or median of the distribution but instead falls near the 30% probability percentile. Thus, the uncertainty estimates are primarily producing values greater than the original base case estimate. The range of values for a 2σ standard deviation is approximately 4.3 to 6.5 log units or two orders of magnitude and 3σ is 3.8 to 6.9 log units or three orders of magnitude. The distribution form is remarkably close to a normal distribution.
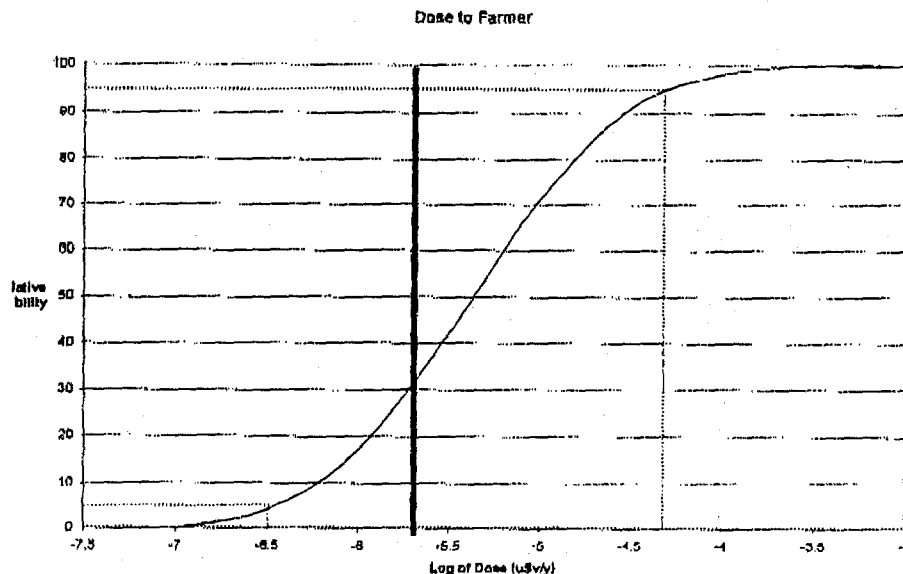

Dose to Farmer
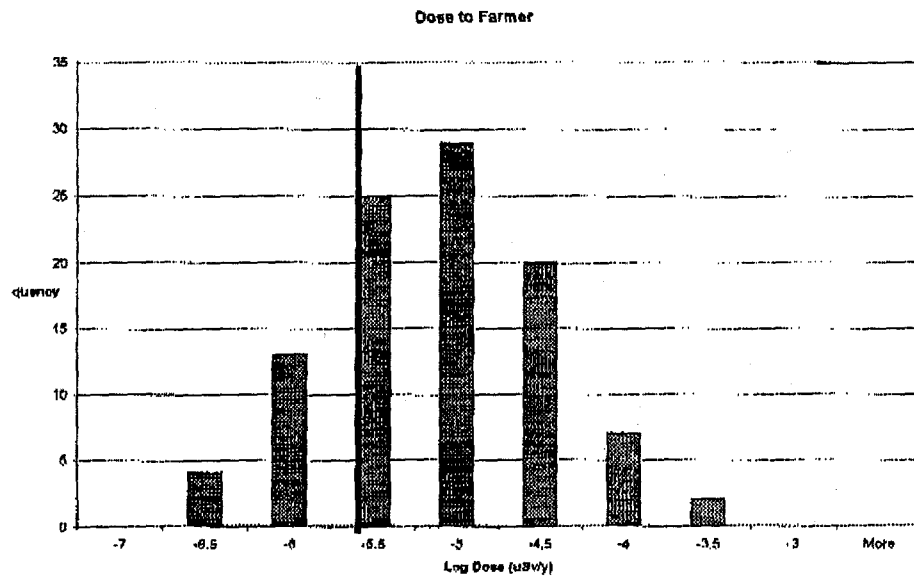
Figure 4. Probability density function of total dose to receptor along with cumulative distribution function.

CONCLUSIONS

The results of this uncertainty assessment confirm that a simplified version of the original model string can be developed using the RIP code to represent the main functions of the original system which runs in significantly less time. This second model development effort also verifies that the original model sequence was being implemented in accordance with the specified conceptual model. The initial results reported in this paper show that it is feasible to implement a full uncertainty assessment and that the current understanding of parameter uncertainty will lead to a significantly wide distribution of uncertainty about the base case results.

ACKNOWLEDGEMENTS

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