

PROBABILISTIC PERFORMANCE ASSESSMENT MODELING USING A MICROSOFT® EXCEL™ WORKBOOK

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ABSTRACT

In the mid-1980s, the United States Department of Energy (DOE) disposed of a small quantity of classified transuranic (TRU) waste in four intermediate depth boreholes at Area 5 of the DOE's Nevada Test Site (NTS). This paper describes a computer program implemented in a Microsoft® Excel™ workbook to perform a probabilistic Monte-Carlo simulation of the movement of these disposed radionuclides and their daughter products toward the land surface. This simulation tracks the movement and cumulative releases of 19 different radionuclides over a 10,000-year regulatory period.

Disposal of TRU waste in these boreholes must comply with U.S. Environmental Protection Agency requirements found at 40 CFR 191 (1), and this regulation contains four general requirements: containment, assurance, individual protection, and groundwater protection. Excepting the qualitative assurance requirement, these requirements are quantitative. The containment requirements prescribe a process that must consider the effects of "all significant processes and events" in estimating cumulative radionuclide releases to the "accessible environment" over 10,000 years. These cumulative releases are compared with probabilistic release limits, making it necessary for the estimated releases to be calculated probabilistically. Probabilistic analyses provide a means of capturing the uncertainty inherent in assessing performance far into the future.

Compliance with the three quantitative requirements of 40 CFR 191 is determined through performance assessments which, because of the nature of the requirements, often use very complicated computer programs that take days to run. However, because of the simplicity of this site and the processes being modeled, two Excel™ workbooks, with code written in Microsoft® Visual Basic™, can implement the performance assessment for the TRU waste in the NTS boreholes. This approach has yielded significant savings in time and money, both in the code development effort and in running the code to produce results.

One workbook produces a complementary cumulative distribution function for assessing compliance with the containment requirements, and the second workbook estimates doses to the

whole body and specific organs for assessing compliance with the individual protection requirements. Assessing compliance with the groundwater protection requirements does not require a workbook or other calculations: 40 CFR 191 requires protection of special sources of groundwater, and the groundwater beneath the NTS boreholes does not meet the definition of special sources of ground water. The containment requirements workbook is driven by a subprocedure that calls 17 other subprocedures and 13 functions. The individual protection requirements workbook is driven by a subprocedure that calls 17 other subprocedures and 18 functions.

Both workbooks use the same radionuclide transport model for the advection, diffusion, and dispersion of dissolved radionuclides up to the ground surface as well as uptake of radionuclides by plants. The transport model also accounts for radioactive decay and production, bioturbation, and adsorption and precipitation/dissolution of radionuclides. Both workbooks perform multiple simulations using sets of parameter values generated by Latin Hypercube sampling. Selected intermediate results and final results are stored in worksheets to facilitate sensitivity analyses and debugging. For the containment requirements workbook, 1,000 simulations can be run in approximately 7 hours while for the individual protection requirements workbook, 125 simulations can be run in approximately 2 hours.

INTRODUCTION

Summary of Greater Confinement Disposal (GCD) Project

In 1981, the DOE's Defense Low-Level Waste Management Program asked the Nevada Operations Office of the DOE (DOE/NV) to demonstrate the feasibility of using Greater Confinement Disposal (GCD) boreholes for disposal of high-specific activity low-level waste (LLW) (i.e., waste packages containing large amounts of tritium). This disposal method used boreholes approximately 10 ft (3 m) in diameter and 120 ft (36.6 m) deep where the waste was placed a minimum of 70 ft (21 m) below the land surface and a minimum of 650 ft (200 m) above the groundwater. The GCD concept was so named because it provides greater confinement than near-surface burial.

The first borehole, the GCD Test (GCDT) borehole, was constructed in the Area 5 Radioactive Waste Management Site of the Nevada Test Site (NTS). GCDT was augured, instrumented, loaded with wastes, and monitored in order to test the GCD disposal concept. Following these tests, twelve more boreholes were augured and used to dispose of additional radioactive wastes including transuranic (TRU) waste. All of the TRU wastes placed in the GCD boreholes are classified for national security reasons and cannot meet the waste acceptance criteria for the Waste Isolation Pilot Plant. At the time of emplacement, TRU waste was governed by Chapter II of former DOE Order 5820.2 (2)[DOE 1984], and this Order required that TRU waste disposal systems meet the U.S. Environmental Protection Agency's (EPA's) requirements for disposal of TRU wastes, which is 40 CFR 191 (1)[EPA, 1985].

DOE/NV contracted with Sandia National Laboratories (SNL) to conduct a technical analysis or Performance Assessment (PA) to determine if the TRU wastes placed in the GCD boreholes meet the requirements set forth in 40 CFR 191. Detailed discussions of the disposal system, regulatory objectives of the analysis, the conceptual models of the transport and exposure

processes, and ensuing analyses are provided in Baer et al., 1994 (3) and Price et al., 1992a and b (4,5). This work is briefly summarized in this report to provide a context for the performance assessment calculations.

Performance Requirements

Subpart B of 40 CFR 191 defines three quantitative requirements that the disposal system must meet: containment, individual protection, and groundwater protection. A fourth set of qualitative requirements (assurance) helps provide confidence that the three quantitative requirements are met.

To meet the Containment Requirement (CR), "[d]isposal systems shall be designed to provide the reasonable expectation, based on performance assessment, that the cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events shall: (a) have a likelihood of less than one chance in 10 of having an EPA Sum greater than one; and (b) have a likelihood of less than one in 1,000 of exceeding an EPA Sum of 10" (40 CFR 191.13). The EPA sum is the ratio of the calculated releases (the calculated curies that move through the controlled area boundary) divided by the number of curies set by the release limit. Release limits are defined in 40 CFR 191. This requirement mandates performance assessment and stipulates that the uncertainties in future system behavior be quantified. 40 CFR 191 is the only probabilistic environmental protection standard in the United States.

To meet the Individual Protection Requirement (IPR), "[d]isposal systems shall be designed to provide a reasonable expectation that, for 1,000 years after disposal, undisturbed performance of the disposal system shall not cause the annual dose equivalent from the disposal system to any member of the public in the accessible environment to exceed 25 millirems to the whole body or 75 millirems to any critical organ" (40 CFR 191.15). This requirement entails an evaluation of the various pathways that might lead a member of the public to be exposed to contamination. Unlike the containment requirement, the individual protection requirement is not explicitly probabilistic.

The Groundwater Protection Requirement (40 CFR 191.16) defines concentration and dose limits for contamination in a special source of groundwater, which apply for 1,000 years after disposal assuming undisturbed performance of the disposal system. Analyses of current recharge conditions conclude that contamination of groundwater under undisturbed conditions is extremely unlikely (3). No additional quantitative analyses are planned to address the groundwater protection requirement.

Overview of Performance Assessment Process

In SNL's methodology, PA is part of an iterative approach to evaluating compliance with regulatory criteria that explicitly treats the uncertainties inherent in the future behavior of the system. In this approach, PA calculations are designed to support regulatory decision making rather than to accurately predict system performance. Specifically, the PA analysis is constructed so that if the results indicate compliance with the quantitative requirements, then the system is very likely to comply. Designing the analysis in this way typically leads to a stylized

representation that conservatively approximates the complex behavior of the actual system. This stylized representation, in turn, leads to mathematical models that are typically much simpler than models designed to mimic details of the system.

For the GCD disposal system, the conceptual model of the “natural conditions” describes the key transport processes that can potentially influence the quantitative regulatory performance measures. This conceptual model leads to a system of one-dimensional advection/dispersion/diffusion equations for contaminants dissolved in liquid pore water and a one dimensional diffusion equation for radon transport in the gas phase. The mathematical model also includes auxiliary relations modeling chemical dissolution and precipitation, uptake and transport of contaminants by plants, and redistribution of contaminants by burrowing animals.

The GCD boreholes are co-located with LLW trenches which have been used for the shallow land burial of LLW. Subsidence of those trenches is expected and will, at a minimum, alter the movement of water in the near surface. Sandia is currently analyzing the movement of water in the vadose zone, given subsidence, precipitation, and assuming a return to cooler and wetter climatic conditions. Some combination of conditions might lead to groundwater recharge. If so, the model will be modified to include the effect of those conditions on overall performance.

CONCEPTUAL MODEL OF THE DISPOSAL SYSTEM

Conceptual Model of Flow and Transport

To assess the performance of the disposal system, it is necessary to make assumptions based on what is known about the system. The purpose of the performance assessment is to estimate radionuclide releases over long periods of time to support a compliance decision regarding 40 CFR 191, not to predict the actual performance of the disposal system. Some assumptions are made because they are reasonable, some are made because they simplify the calculations, some are realistic assumptions, and some are made because they are conservative. Conservative, in this context, means that the estimated radionuclide release to the accessible environment will not be reduced because of the assumption.

The conceptual model comprises the simplifying assumptions about the system behavior that underlie the performance assessment calculations. These assumptions have been developed from a diverse and extensive body of information about the site. This information includes basic site data as well as models developed to test alternative hypotheses about system behavior. The current conceptual model of the GCD disposal system, including the evidence supporting this conceptual model, is described in Baer et al. 1994 (3). This conceptual model is summarized below to provide the basis for the mathematical models and parameters used in the performance assessment calculations.

The conceptual model of water movement and contaminant movement for the GCD disposal system is illustrated in Figure 1. Current climate conditions at the site result in a hydrologic system dominated by evapotranspiration (i.e., infiltrating water is rapidly recycled to the atmosphere and does not infiltrate past the near surface). The upper 3 to 10 feet (1 to 3 meters) of native alluvium is hydrologically active. Water content and the magnitude and direction of fluxes are influenced by several factors including episodic infiltration, evaporation, root uptake

and the activities of burrowing animals and insects (bioturbation). Below 10 feet (3 meters) to a depth of approximately 16.5 feet (5 meters), root and animal activity diminish but can still occur.

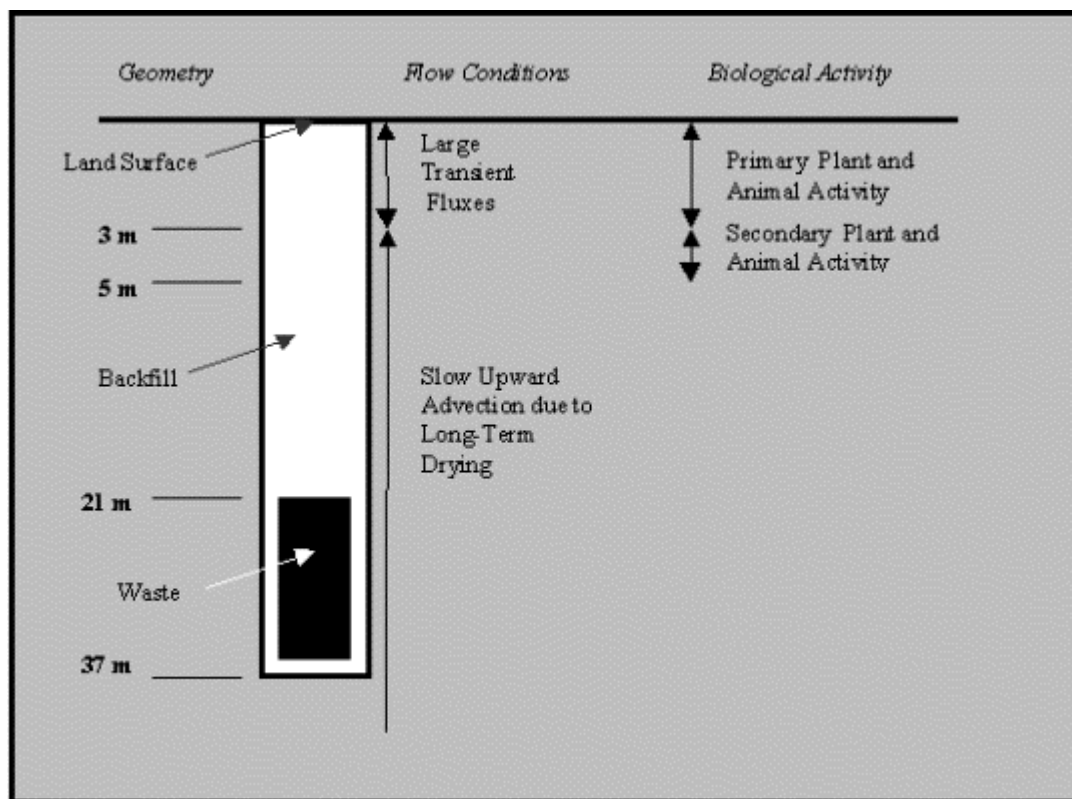
Between a depth of 10 to 115 feet (3 - 35 meters), the alluvium shows increasing matric potential with depth, indicating a steady and very slow upward flux of pore water. This upward flux is based on the pore water in the alluvium responding to the current arid climate, since past climates produced wetter conditions in the alluvium.

Near the surface, weather-induced intermittent variations of matric potential are superimposed on this annual mean matric potential inducing upward and downward flow of water. The bottom of this zone can be thought of as a "no-flux" liquid phase boundary based on the net effect of this transient cycling. The only moisture that passes this boundary is that which is imbibed by plants or moved by burrowing animals.

Transport processes important for the disposal system include diffusion of gaseous radionuclides, upward liquid-phase advection, dispersion and diffusion of solutes in the pore water, plant uptake and bioturbation due to plant and animal/insect activity, adsorption, precipitation and radioactive decay and production.

The alluvium through which radionuclides are transported is homogeneous and isotropic. Hydraulic conditions in the backfill are assumed to be identical to those in the alluvium. Groundwater flow upwards is steady-state. Moisture content is constant spatially and temporally. Waste packages are assumed to offer no isolation, and to be breached at the time of disposal. The source of radionuclides is continuously altered by dissolution and by radioactive decay and production throughout the simulation time.

Concentrations of radionuclides in plants are assumed to be linearly proportional to their total concentration in soil. Radionuclide mass is transported past the land surface through plant growth and decay. In a given time period, bioturbation is assumed to transport some fraction of the soil mass at a given depth (and any radionuclides in the soil) to the land surface. The fraction of soil transported to the land surface in a given period is a function of depth.



Over the 10,000 year performance period for the CR, the climate at the NTS is expected to change to an extent that the performance of the disposal system might be affected. The most likely change would lead to slightly cooler and wetter conditions at the site (6). This shift in climate is assumed to cause a change in the type and density of plants growing over the boreholes.

Conceptual Model of Exposure

The performance measure of the IPR is dose to a member of the public (MOP). The analysis must consider the conditions under which the MOP might become exposed to radioactive waste. Both the Nuclear Regulatory Commission (NRC) and the DOE are responsible for approving of LLW performance assessments. As a result, both DOE (7) and NRC (8) have developed reasonable but conservative exposure conditions that serve as surrogates for unknowable future exposures. Two significant differences between IPR and LLW exposure conditions are that: 1) the IPR is for undisturbed conditions only, meaning that well cuttings and basements do not contribute to dose, and 2) the IPR dose is based on only those radionuclides that have reached the accessible environment.

Tailoring the LLW disposal exposure conditions proposed by the DOE and NRC to the IPR led to the following exposure conditions:

1. The MOP lives in a house near all four boreholes.

2. The house may have a basement, but the basement does not contribute to the dose.
3. The MOP has a garden, which is also near the boreholes. The garden is the source of contamination for all exposure mechanisms. Leafy vegetables, root vegetables, fruits, grains, and hay are grown in the garden.
4. The individual spends about a fifth of his time outdoors, working in the garden and at other activities near the house.
5. Contamination of the garden soil occurs as radionuclides are transported in the wind from the ground surface above the boreholes to the nearby garden.
6. The MOP is exposed by inhaling radionuclides that are suspended in the air, ingesting contaminated soil, ingesting contaminated produce from the garden, ingesting contaminated animal products, and by external exposure from the ground surface and from immersion.

MATHEMATICAL MODEL OF TRANSPORT FOR THE DISPOSAL SYSTEM

A mathematical model is required in order to calculate the integrated discharge from the disposal system for the CR, and to calculate potential dose for the IPR. The development of the mathematical model, leading to a numerical approximation, is detailed in Cochran et al. 1998 (9). The model is summarized here to explain the basis of the numerical approximation implemented in the workbooks.

The disposal cell and overlying backfill are divided into a number of regions. Based on the conceptual model, the mass density of a dissolved radioactive contaminant i in each of these regions is described by a conservation equation which includes advection, diffusion, and dispersion in the flowing pore water, radioactive production and decay, uptake by plants, and bioturbation:

$$\frac{d m_i^x}{dt} = \frac{q_i^{x-1}}{L^x} - \frac{q_i^x}{L^x} - q_{dist,i}^x + \lambda_{i-1} m_{i-1}^x - \lambda_i m_i^x \quad (\text{Eq. 1})$$

where:

- | | | |
|-------------|---|--|
| m_i^x | = | mass density of radionuclide i in transport region x (moles/m ³ alluvium), |
| t | = | time (yr), |
| q_i^{x-1} | = | flux of radionuclide i out of transport region $x - 1$ into the overlying transport region x (moles/m ² alluvium yr), |
| q_i^x | = | flux of radionuclide i out of transport region x into the overlying transport region $x+1$ (moles/m ² alluvium yr), |
| L^x | = | height of transport region x (m), |

- $q_{dist,i}^x$ = flux of radionuclide i out of transport region x due to distributed sinks such as plant uptake and bioturbation (moles/m³ yr),
 λ_i = decay constant for isotope i , $\lambda_i = \ln(2)/t_{1/2}$, (1/yr).

The flux of radionuclide i out of transport region x and into transport region $x + 1$ is a result of advection, dispersion, and diffusion. This flux can be approximated by:

$$q_i^x = q_l (\gamma C_i^x + (1-\gamma) C_i^{x+1}) - \left(\frac{\alpha q_l + D_m / \tau}{(L^x + L^{x+1}) / 2} \right) (C_i^{x+1} - C_i^x) \quad (\text{Eq. 2})$$

where:

- q_l = liquid phase advective flux density (m³ water/m² alluvium yr),
 $\bullet$ = upstream weighting factor for evaluating advective concentration (dimensionless)
 C_i^x = concentration of radionuclide i in pore fluid (moles/m³ water).
 $\bullet$ = longitudinal dispersivity (m),
 D_m = molecular diffusion coefficient (m²/yr),
 $\bullet$ = tortuosity (dimensionless).

Contaminants are assumed to be subject to an isotope-specific solubility limit, so that the mass densities and dissolved concentrations are related by:

$$C_i^x = \min \left(\frac{m_i^x}{R_i \theta}, C_{i,sol} \right) \quad (\text{Eq. 3})$$

where:

- $C_{i,sol}$ = isotopically apportioned solubility of radionuclide i (moles/m³ water).
 R_i = retardation coefficient of radionuclide i (dimensionless).
 θ = volumetric moisture content (dimensionless)

Contaminant flux across the bottom of the waste cell is assumed to be zero. As discussed above, contaminants transported towards the land surface are ultimately removed by plant uptake, bioturbation, or fall out of solution as the pore water evaporates. This process is modeled by requiring that the contaminant flux across the upper boundary of some specified region is zero.

An approximate solution, at a sequence of evaluation times, can be obtained using a semi-implicit approximation for the time derivative:

$$\begin{aligned}
& -\Delta t \omega A_D^x C_{i,n+1}^{x-1} + (1 + \Delta t \omega B_M^x) m_{i,n+1}^x + \Delta t \omega B_C^x C_{i,n+1}^x - \Delta t \omega A_U^x C_{i,n+1}^{x+1} \\
& = \Delta t (1 - \omega) A_D^x C_{i,n}^{x-1} + (1 - \Delta t (1 - \omega) B_M^x) m_{i,n}^x - \Delta t (1 - \omega) B_C^x C_{i,n}^x + \Delta t (1 - \omega) A_U^x C_{i,n}^{x+1} \\
& \quad + \Delta t (\lambda_{i-1} ((1 - \omega) m_{i-1,n}^x + \omega m_{i-1,n+1}^x) - a_i^x)
\end{aligned} \tag{Eq. 4}$$

where:

- ω = weighting factor for rate terms evaluated at the end of the timestep implicate terms)

$$A_D^x = \frac{\gamma q_l + q_D^{x-1}}{L^x}$$

$$A_U^x = \frac{q_D^x - (1 - \gamma) q_l}{L^x}$$

$$B_{Mi}^x = b_i^x + \lambda_i$$

$$B_C^x = B_D^x + B_U^x$$

$$B_D^x = \frac{(\gamma - 1) q_l + q_D^{x-1}}{L^x}$$

$$B_U^x = \frac{\gamma q_l + q_D^x}{L^x}$$

$$q_D^x = \frac{\alpha q_l + D_m / \tau}{(L^x + L^{x+1}) / 2}$$

$$q_{dist,i}^x = a_i^x + b_i^x m_i^x$$

The mass density of radon is described by a conservation equation which includes advection and diffusion in the air-filled pore spaces, radioactive production and decay:

$$\frac{d m_{Rn}^x}{dt} = \frac{q_{Rn}^{x-1}}{L^x} - \frac{q_{Rn}^x}{L^x} + \lambda_{Ra} m_{Ra}^x - \lambda_{Rn} m_{Rn}^x \tag{Eq. 5}$$

where:

$$\begin{aligned} m_{Rn}^x &= \text{mass of radon in control volume } x \text{ (moles/m}^3\text{)}, \\ q_{Rn}^x &= \text{flux of radon out of control volume } x \text{ (moles/m}^2 \text{ yr)} \\ \lambda_{Ra} &= \text{decay constant for radium (1/yr),} \\ m_{Ra}^x &= \text{mass of radium in control volume } x \text{ (moles/m}^3\text{)} \end{aligned}$$

$$q_{Rn}^x = \frac{2 D_{Rn}}{L^x + L^{x+1}} (C_{Rn}^x - C_{Rn}^{x+1})$$

$$\begin{aligned} \lambda_{Rn} &= \text{decay constant for radon (1/yr).} \\ D_{Rn} &= \text{diffusion coefficient for radon (m}^2\text{/yr), and} \\ C_{Rn} &= \text{concentration of radon in control volume } x \text{ (moles/m}^3 \text{ of air).} \end{aligned}$$

The concentration of radon in transport region x , C_{Rn}^x , is related to the mass density of radon

$$C_{Rn}^x = \frac{m_{Rn}^x}{\epsilon} \quad (\text{Eq. 6})$$

in transport region x , m_{Rn}^x ,

where:

$$\bullet \quad = \quad \text{air-filled porosity of the alluvium (dimensionless).}$$

A similar numerical approximation yields radon mass densities at a sequence of specified time steps:

$$\begin{aligned} & -\Delta t \omega \frac{A_D^x}{\epsilon} m_{Rn,n+1}^{x-1} + (1 + \Delta t \omega (B_M^x + \frac{B_C^x}{\epsilon})) m_{Rn,n+1}^x - \Delta t \omega \frac{A_U^x}{\epsilon} m_{Rn,n+1}^{x+1} \\ & = \Delta t (1 - \omega) \frac{A_D^x}{\epsilon} m_{Rn,n+1}^{x-1} + (1 - \Delta t (1 - \omega) (B_M^x + \frac{B_C^x}{\epsilon})) m_{Rn,n}^x + \Delta t (1 - \omega) \frac{A_U^x}{\epsilon} m_{Rn,n}^{x+1} \\ & \quad + \Delta t \lambda_{Ra} ((1 - \omega) m_{Ra,n}^x + \omega m_{Ra,n+1}^x) \end{aligned} \quad (\text{Eq. 7})$$

where:

$$A_D^x = \frac{q_{D_{Rn}}^{x-1}}{L^x}$$

$$A_U^x = \frac{q_{D_{Rn}}^x}{L^x}$$

$$B_M^x = \lambda_{Rn}$$

$$B_C^x = A_D^x + A_U^x$$

$$q_{D_{Rn}}^x = \frac{2 D_{Rn}}{(L^x + L^{x+1})}$$

MODEL IMPLEMENTATION AS SPREADSHEET MACROS

This simple mathematical model defined by Equations 4 and 7 was implemented as Microsoft® Visual Basic™ modules in an Excel™ workbook. This approach offers a number of advantages during model development, testing, application, and documentation of the model. The interconnections among the elements of the analysis can be directly traced through the workbook. A particular benefit for the PA is that the analysis is almost entirely self-contained: the input data, model code, results, and graphics are available in one document. This format allows the document to be distributed to a broad audience for review. The workbook format allows the information used in the PA to be easily browsed and displayed, facilitating review and interpretation. The workbook implementation represents a significant saving in time and money, both in the code development effort and in running the code to produce results.

Separate workbooks implement the system models to address the CR and the IPR. The Monte-Carlo analysis used for both requirements entails a large number of calculations, but the simple model structure allows acceptable performance when these calculations are implemented as spreadsheet macros. One workbook produces a complementary cumulative distribution function for assessing compliance with the CR, while the second estimates doses to the whole body and specific organs for assessing compliance with the IPR. The containment requirement workbook contains 38 spreadsheets and is driven by a subprocedure that calls 17 other subprocedures and 13 functions. The individual protection requirements workbook contains 57 spreadsheets and is driven by a subprocedure that calls 17 other subprocedures and 18 functions.

Figure 2 illustrates the transport and exposure processes simulated in the workbook models along with the important system properties. Both workbooks have the same radionuclide transport model, based on Equation (4), that simulates mobilization of the waste, advection, diffusion, and dispersion of dissolved radionuclides up towards the ground surface, and transport of radionuclides to the ground surface by plant uptake and animal burrowing. The common transport model also includes radioactive decay and production, adsorption, and chemical precipitation of radionuclides.

The two workbooks differ in their use of the calculated radionuclide discharge. The containment requirement workbook integrates the radionuclide flux over a 10,000 year performance period. A weighted sum over all radionuclides is then calculated for comparison against the regulatory

requirement. The workbook model for the individual protection requirement accumulates all discharged radionuclide mass over a 1,000 year performance period. All of this mass is assumed to be transferred to the MOP's garden. The exposure model then calculates the dose resulting from the garden soil contamination due to diverse ingestion, inhalation, and external exposure pathways.

Figure 3 illustrates the flow of information through the performance assessment process, including parameter definition, parameter sampling, system simulation, and performance measure calculation. This figure generally applies to both workbook models. Both workbooks perform multiple simulations using multiple sets of parameter values generated using Latin Hypercube sampling (LHS) (10). The sample parameter values generated by LHS are imported into a spreadsheet in the workbook. The transport model is then executed for each of the parameter sample sets in the spreadsheet. Probability distributions for integrated release and dose are assembled from these repeated simulations. Selected intermediate results and final results are stored in auxiliary spreadsheets to facilitate sensitivity analyses and to help in interpreting and debugging the calculations.

As Figure 3 illustrates, much of the PA information flow takes place within the workbooks, and is readily available for review using the standard display tools for the spreadsheets in the workbook. The workbook models contain most of the information used in the PA, including the code that implements the transport and exposure calculations. This self-contained approach benefits PA by making the assessment easier to design, debug, review, document, and analyze than more traditional approaches. This implementation helps make the calculations transparent and verifiable, but has some cost in computational efficiency. Because of the simplicity of the model, however, the execution time for a set of parameter samples is quite acceptable: for the CR workbook, 1,000 simulations can be run in approximately 7 hours; for the IPR workbook, 125 simulations can be run in approximately 2 hours.

STATUS AND EXAMPLE RESULTS

The workbook models are currently being verified and validated as part of the quality assurance process for the final GCD PA. This process includes review of the underlying mathematical model, review of the implementing code, and comparison of the model results to analytical solutions where appropriate. The model input parameters are also being reviewed and verified in preparation for the final PA calculations. Additionally, Sandia is currently analyzing the movement of water in the vadose zone, given subsidence, precipitation, and assuming a return to cooler and wetter climatic conditions. These analyses may alter the conceptual model of the disposal, which may in turn require modification of the workbook models. The current versions of the workbooks and the current values and distributions for input parameters were used to produce the example results discussed below.

The CR model uses more than 100 input parameters to characterize the disposal system. Of these, 63 are considered to be uncertain, and are assigned probability distributions based on the existing state of knowledge. The IPR model uses more than 200 input parameters, 92 of which are considered to be uncertain. For both models, parameters that are not considered uncertain are

assigned fixed values based on generally accepted sources (such as radionuclide half-lives) regulatory stipulation, or convention (such as the exposure period of a resident farmer).

Cochran et al. (9) contains a complete description of the input parameters along with an explanation for the constant values or distributions used in the analysis. A discussion of each of the input parameter values is outside of the scope of the present document. Therefore, a complete list of the input parameters, and the values used in the analyses, are not summarized here; interested readers are referred to Cochran et al. Table 1 lists some of the input parameters that are assigned fixed values in the analysis. These parameters are stored in the "Geometry" spreadsheet in the workbook models, and define the dimensions of the disposal system and certain behavioral properties of the exposed individual. Uncertain input parameters are described by probability distributions. Table 2 lists some of the uncertain parameters used in the transport model common to both workbooks.

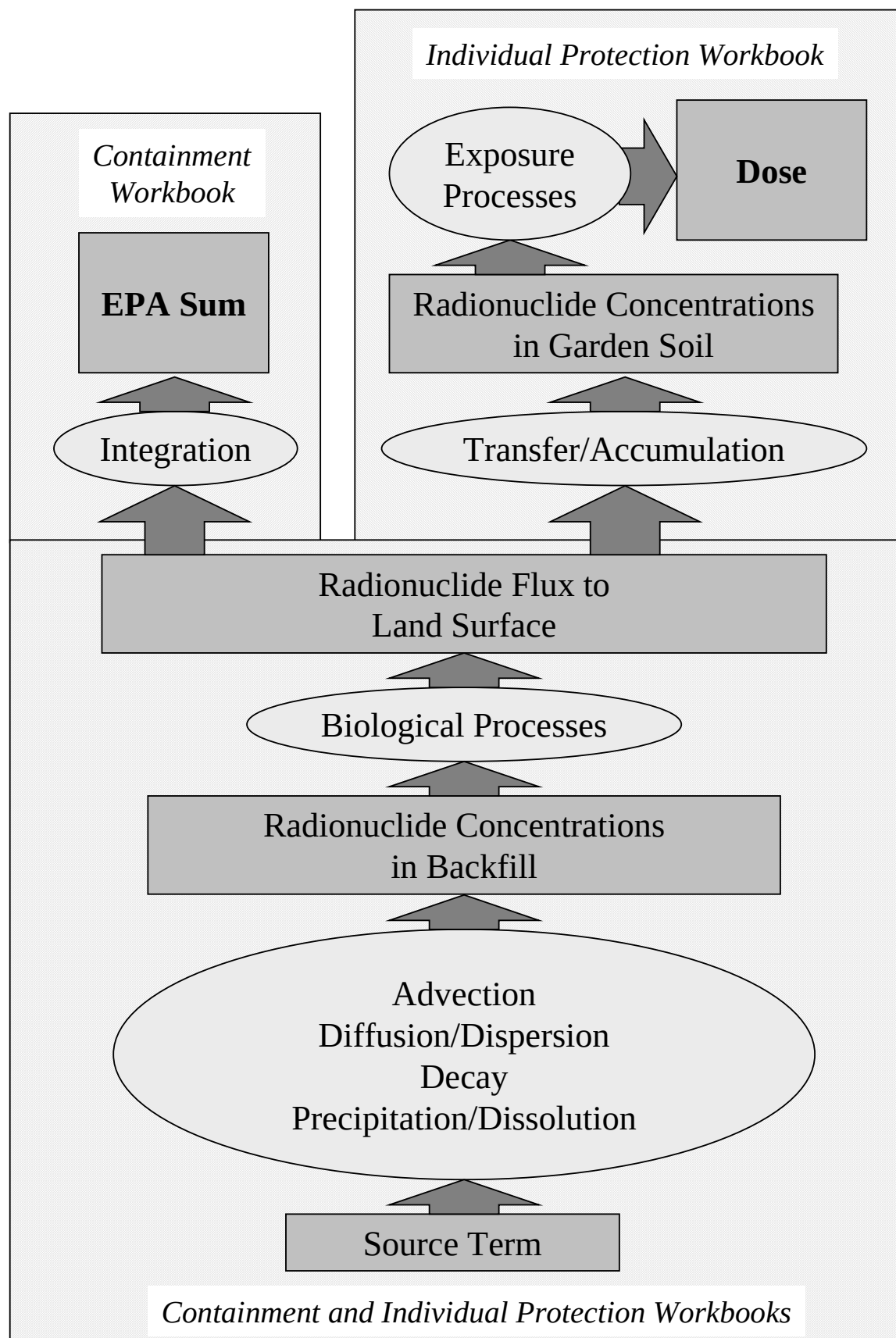


Figure 2 - Disposal System Processes and Properties Included in the Workbook Models

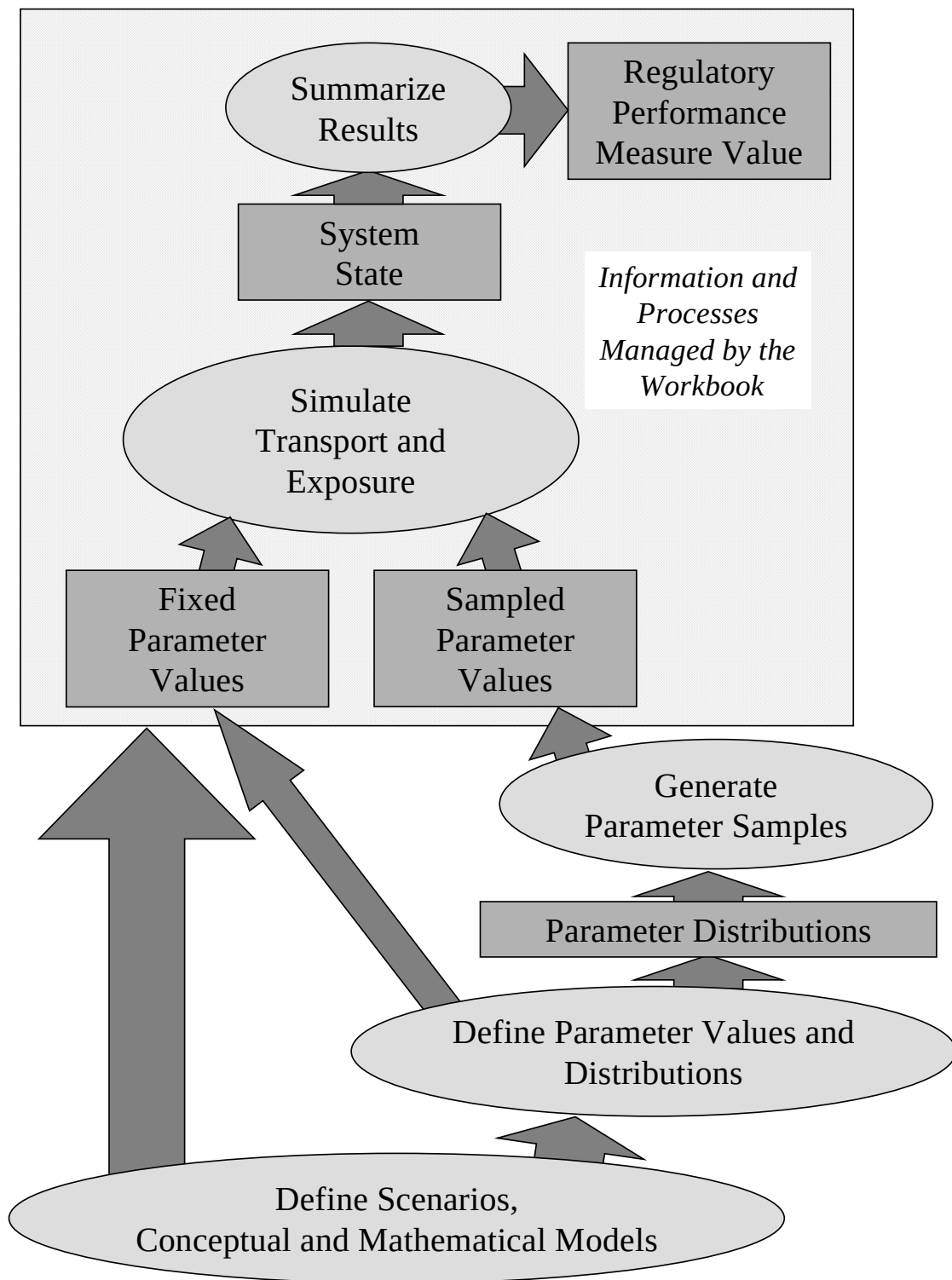


Figure 3 - Key Processes and Information Flow in Performance Assessment Modeling

Table 1 - Selected Deterministic Input Parameters for the Individual Protection Workbook Model

<i>Parameter Description</i>	<i>Units</i>	<i>Value</i>
Disposal_Area	m	35
Borehole_Height	m	15.2
Bioturbation_Depth	m	1
Porosity	none	0.35
Breathing_Rate	m ³ /y	8000
Dust_Loading	kg/m ³	1x10 ⁻⁷
Time_Outdoors	y/y	0.205
Time_Indoors	y/y	0.795
Indoor_Airborne_Shielding_Factor	none	0.4
Indoor_External_Shielding_Factor	none	0.7
Average_Wind_Speed	m/s	2
Molecular_Diffusion_Coefficient	m ² /y	0.0316
Radon_Diffusion_Coefficient	m ² /y	113
Mixing_Height	m	2
Garden_Depth	m	0.15
Garden_Area	m ²	2511
Human_Intake_Rate_Leafy	kg/y	64
Human_Intake_Rate_Root	kg/y	216.8
Human_Intake_Rate_Fruit	kg/y	114.4
Human_Intake_Rate_Grain	kg/y	124.8
Human_Intake_Rate_Beef	kg/y	52.6
Human_Intake_Rate_Poultry	kg/y	29.2
Human_Intake_Rate_Eggs	kg/y	8.3
Human_Intake_Rate_Milk	l/y	310
Human_Intake_Rate_Water	l/y	730
Human_Intake_Rate_Soil	kg/y	0.0365
Crop_Yield_Feed_Hay	kg/m ²	1
Crop_Yield_Feed_Grain	kg/m ²	1
Crop_Yield_Leafy	kg/m ²	2
Crop_Yield_Root	kg/m ²	4
Crop_Yield_Fruit	kg/m ²	2
Crop_Yield_Grain	kg/m ²	1

Table 2 - Selected Uncertain Input Parameters for the Individual Protection Workbook Model

<i>Parameter Description</i>	<i>Units</i>	<i>Distribution</i>
Specific_Discharge	m/y	Uniform from 1×10^{-5} to 9×10^{-4}
Moisture_Content	None	Uniform from 0.05 to 0.15
Am_Solubility	Molal	Loguniform from 4×10^{-9} to 2×10^{-6}
Am_Kd	m^3/kg	Lognormal from 1×10^{-6} to 5×10^{-3}
Am_Concentration_Ratio_Leafy	None	Lognormal from 3×10^{-5} to 1
Am241_Inventory	Moles	Uniform from 8×10^{-2} to 1×10^{-1}

For both models LHS was used to produce a set of samples of the input parameter values, and the performance assessment model was executed in turn for each of these parameter sets. For each of the set of sampled values for the uncertain input parameters, the workbook model calculates the integrated release (for the CR) or the dose to the MOP (for the IPR). For the CR, the distribution of possible integrated releases is explicitly required by the regulation. A dose distribution is not explicitly required by the IPR, however, the input parameter values are still uncertain, and characterizing the effect of this uncertainty on the regulatory performance measure is good practice. Figure 4 shows example results from the workbook models: the distribution of integrated releases calculated by the CR model and the cumulative distribution function for whole body dose calculated by the IPR model. The integrated release distribution is plotted as a complementary cumulative distribution function (CCDF) which is the probability of the EPA sum exceeding the ordinate (x-axis) value.

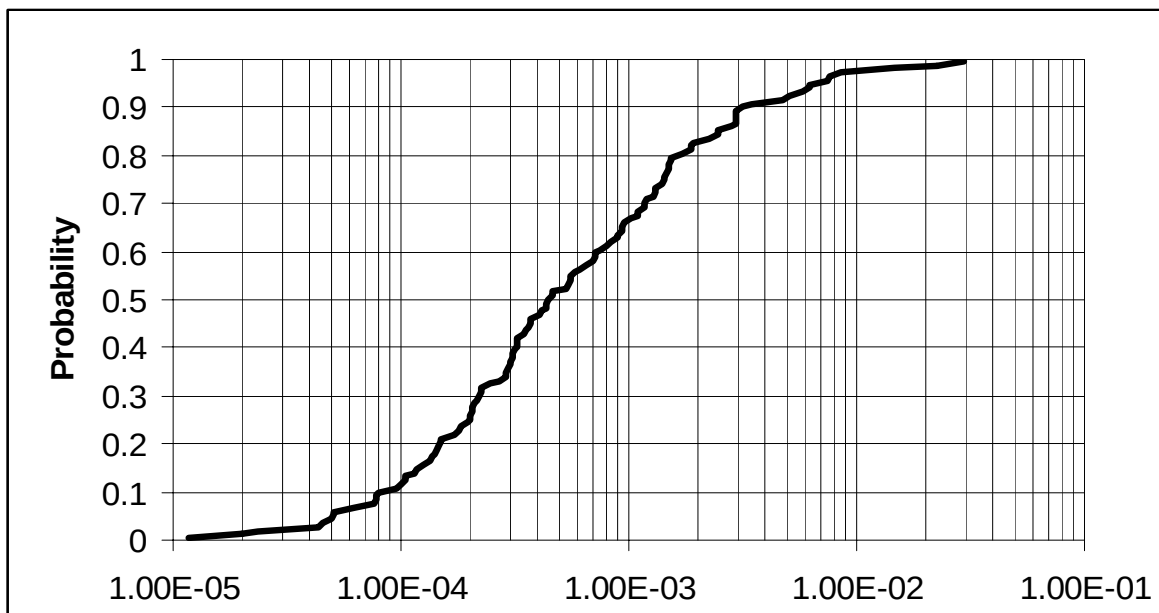
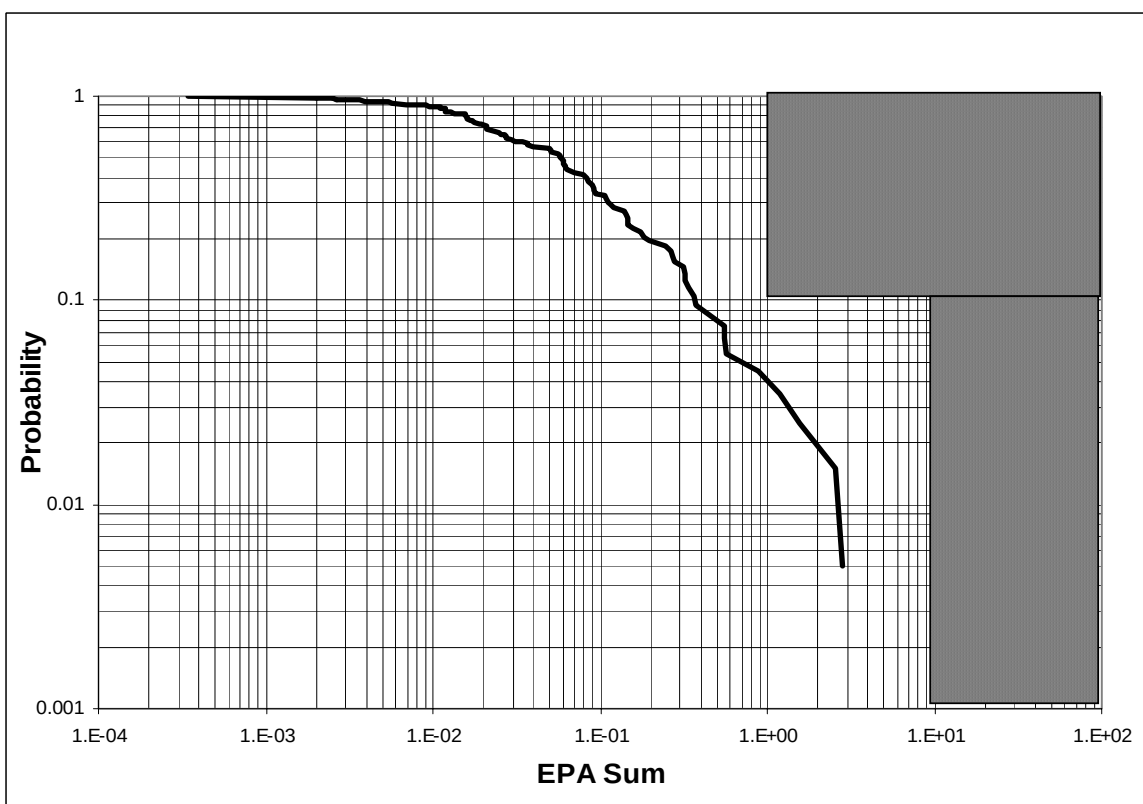
CONCLUSION

Performance assessment calculations are often based on complicated representations of the disposal system. These complex representations can provide high-resolution predictions about the simulated system, but their complexity can make them difficult to justify and costly to implement. Computational demands are compounded when uncertainty in system performance must be quantified.

The PA for the GCD concept against 40 CFR 191 employs a relatively simple computational model. This simplicity results from inherent features of the system, but it is also a consequence of SNL's approach to PA where the model is designed to be a sufficient basis for regulatory decision making given the existing state of knowledge. This approach naturally requires simplifying conservative assumptions about uncertain aspects of system behavior.

The simplicity of the performance assessment models allowed use of Microsoft® Visual Basic™ macros in an Excel™ workbook as a viable, low cost implementation. This approach provided a

convenient environment for developing, debugging, and testing the implementing code. The computational simplicity of the model also provided for acceptable simulation times in spite of the relative inefficiencies of the implementing language. Apart from computational considerations, this approach provides significant advantages for performance assessment applications in particular. The resulting workbook is a nearly self-contained analysis, containing the input parameter values, descriptions of distributions, computational modules, results, and graphics. Information links within the workbook insure consistency of input and results leading to an analysis that is largely self-documenting. The widespread availability of Excel™ allows the analysis to be easily distributed for review and allows reviewers to explore the performance consequences of alternative assumptions or parameter values. These features directly contribute to performance assessment by helping to develop confidence in the implementation of the performance assessment models and in the resulting regulatory decisions.



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