

PROBABILISTIC METHODS FOR ASSESSING LONG-TERM PERFORMANCE^a
OF HIGH-LEVEL WASTE PACKAGES

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ABSTRACT

Probabilistic methods are attractive for assessing the performance of high-level waste packages. This paper presents several probabilistic methods, along with examples illustrating how the calculations are performed. Global simulation, modular simulation, and a cascade approach are examined, and plans for comparing the predictions of these approaches in the future are discussed.

INTRODUCTION

The Aerospace Corporation is assisting the Nuclear Regulatory Commission in identifying and developing methods to be used in independently assessing the performance of Department of Energy high-level radioactive waste packages in a permanent underground repository.

Early in the project, a number of performance assessment methods were reviewed. After careful consideration of the necessary attributes of performance assessment to be used as part of the licensing process, it was concluded that the methods should be essentially probabilistic. The probabilistic methods covered in this paper—global simulation, modular simulation, and cascading—represent the approaches considered most attractive for further examination.

ASSESSMENT REQUIREMENTS

As a minimum requirement, a method for assessing the performance of high-level waste packages must be capable of determining whether the licensing criteria will be met. Consequently, a method must be capable of addressing the quantitative performance criteria as stated in the Code of Federal Regulations covering the Nuclear Regulatory Commission¹ and the Environmental Protection Agency.² Currently, these criteria relate to the period of complete containment (300 to 1000 yr) and the maximum and cumulative release rates after the containment period. Because the containment period and post-containment release rates depend on a variety of physical processes, a performance assessment method must incorporate models of these processes as they occur within the package. Because container lifetime depends on temperature, radiation, various chemical processes, and stress, a reasonably complete container lifetime assessment method would include thermal, radiation shielding, radiolysis, groundwater chemistry, corrosion, and stress models. In order to address post-containment

release rates, waste form dissolution and radionuclide transport models would also be included.

To apply all these models, a large data base of material properties must be available. The models and data base of input parameters are the key elements of a performance assessment method. An important aspect of any method is the manner in which the models interrelate, i.e., their coupling. For example, in the corrosion model, the corrosion rate may depend on temperature, but the dependence of thermal conductivity on corrosion might not be taken into account.

PROBABILISTIC METHODS

The use of a probabilistic method for waste package performance assessment is a natural consequence of the large uncertainties regarding both the physical processes and material properties that determine waste package lifetimes and release rates. Recognizing this, the Nuclear Regulatory Commission requires that these uncertainties be addressed.³ A variety of possible approaches with varying levels of complexity are available for dealing with these uncertainties. In one approach, an examination of extreme values, i.e., some type of limit analysis, could be attempted. There is also a large body of mathematical statistics, probability theory, and reliability engineering applicable to problems of this type, and in many cases, these methods can provide valuable additional information and insights regarding waste package performance. With such methods, it is possible to examine not only extreme values, but intermediate values as well, and determine the effects of differences in their relative likelihood. For example, as the degree of knowledge regarding an input parameter improves, the extreme values could become less likely, and this improved knowledge could be reflected in the performance predictions. Thus, not only the range but the relative likelihood of various waste package lifetimes within that range can be predicted and compared. In this paper, the term "probabilistic method" will be limited to methods of this type, and the remaining discussion will be limited to such methods.

For performance assessment, it is frequently convenient to consider a waste package to be a

^aThis work was supported by the U.S. Nuclear Regulatory Commission under Contract No. F04701-83-C-0085. We wish to acknowledge the contributions of A. Bruce Crane to the development of the modular approach.

collection of barriers. The packing and container can be regarded as barriers to the incoming groundwater, the wasteform as a barrier to radionuclide dissolution in the groundwater, and the packing as a barrier to radionuclide release from the waste package. Using this framework, it is possible to classify probabilistic waste package performance assessment methods according to the degree of independence or interaction between the barriers. In this discussion, three basic approaches are distinguished: (1) global simulation in which a single integrated model of the system is used, (2) modular simulation in which the barriers are decoupled and treated independently, and (3) a cascade approach in which some of the most important features of barrier coupling are linked and are passed from one module to the next. These approaches and their advantages and disadvantages are discussed below.

GLOBAL SIMULATION

General Features

A global simulation is the most straightforward approach to assessing waste package performance, but at the same time, it may be the most complex. In its purest form, a global model would be a single, fully integrated model of the system in which all relevant processes, events, and failure modes would be included. No simplifying assumptions would be made regarding interactions among processes and events. However, as the number of processes considered increases, such global models can become large and complex, which results in compromises. This problem occurs frequently in general simulation approaches, and often greatly simplified descriptions of the processes that contribute to system failure are used. Thus, if field equations are required, one-dimensional approximations are substituted for three-dimensional descriptions, and where processes are coupled, independence is assumed.

The large number of random parameters that must be sampled jointly is a problem with the global model approach. Generally, each unknown parameter must be sampled according to a probability distribution characterizing its uncertainty. Global models that essentially use all the parameters jointly require very large numbers of simulation runs because of the large number of combinations of parameter values that must be explored. To reduce the number of runs, it may be necessary to use an efficient sampling strategy, such as stratified or Latin Hypercube Sampling in some of the more complex global models.

Example of a Global Model

An example of a global type of model is the Waste Package Performance Assessment (WAPPA) code,⁴ which is intended to predict the radionuclide containment performance of a complete waste package design, including the packing, all solid barriers, air gaps, and the wasteform. WAPPA uses a set of infinitely long, concentric cylinders to simulate the geometry of the wasteform and surrounding barriers. This simplifies the calculations considerably because the equations for heat flow, stress, and diffusion have closed-form solutions for this geometric configuration. This means that WAPPA is basically a one-dimensional radial model. The WAPPA code consists of a system model, or driver, and five physical process models: radiation, thermal, mechanical, corrosion, and leach/transport. WAPPA is barrier-integrated and process sequential. That is, at any specified time, the closed-form equations governing a single process

are solved simultaneously for all the affected waste package components. However, the processes are addressed sequentially (i.e., the radiation model is called on first, followed by the thermal, mechanical, corrosion, and leach/transport models).

As originally written, WAPPA is not a probabilistic model. However, to demonstrate the use of a global model in a probabilistic calculation, a limited example calculation of a probability density function (pdf) for waste package lifetime was performed using portions of WAPPA. To simplify and expedite the calculations, only WAPPA's thermal and mechanical models were used in the example calculation. The example is intended only to demonstrate the methodology for randomizing a deterministic model and should not be considered an actual performance assessment.

For this example, the chosen barriers were the packing and container, and the waste package lifetime calculation was terminated upon penetration of the container by incoming groundwater. The specific waste package design chosen for the demonstration was the Westinghouse⁵ commercial high-level waste (CHLW) conceptual design for basalt. This design is outdated in that the Basalt Waste Isolation Project (BWIP) intention is to use the short borehole design as its future reference design⁶ and used this design in the Draft Environmental Assessment.⁷

A standard Monte Carlo technique (without stratification) was used to generate the input parameters for the demonstration calculation. Randomized values of seven input parameters were used in repeated WAPPA calculations of the temperatures and stresses in the barriers. The randomized parameters for the demonstration included repository resaturation time, repository hydrostatic pressure, densities of dry and wet packing, and three of the parameters used in computing the corrosion rate. To simplify the calculations, no attempt was made to represent the uncertainties in all the input parameters. Lognormal distributions were assumed for all randomized parameters. However, this choice was largely a matter of convenience. A further examination of the experimental data is needed to identify the most appropriate distributions for the input pdf's.

The densities of dry and wet packing were used to compute its thermal conductivity before wetting and after complete saturation by the groundwater (intermediate degrees of saturation were not addressed). The density of dry packing was also used to compute its hydraulic conductivity. The packing hydraulic conductivity was then used to determine the time from repository resaturation to wetting of the container using the randomized value of hydrostatic pressure. The methodology and equations used for determining the thermal and hydraulic conductivities of the packing from its composition, density, and the properties of its constituents are described in Ref. 8. The calculations were performed in a short subroutine that was added to WAPPA. The original version of WAPPA does not have a packing infiltration model. Instead, it assumes the packing is saturated at some time specified by the user.

WAPPA computes the general corrosion rate from a rate-versus-temperature table provided in one of its data libraries. This procedure was bypassed, and the container corrosion rate, CR (10^{-6} m/yr), was computed using the following chemical reaction equation:

$$CR = K \sqrt{(I_4 - PH)} (PO_2)^{3/2} e^{-2850/T} \quad (1)$$

where K = randomized multiplicative constant,
 PH = randomized pH of groundwater,
 PO₂ = randomized oxygen partial pressure (ppm), and
 T = temperature (degrees Kelvin).

Equations of this general form have been used to describe oxidative corrosion of metals in other unrelated situations. Although there is no justification for applying this particular equation to container corrosion, it contains random variables generally observed or expected to affect the rate of corrosion. Consequently, it afforded the opportunity to demonstrate that such an equation can be used with pdf's and was chosen for this reason alone.

The container was assumed to fail when the stress reached the maximum allowable stress for 1025 carbon steel (15 ksi), which is conservative because the yield stress is about twice the maximum allowable. However, the stress calculation does not include discontinuity stresses.

A large amount of input data was required to perform the calculations, and some of these data are highly uncertain or even unavailable. For example, a value for the yield stress of the basalt/bentonite mixture used for the packing material could not be located. Similar difficulties were encountered in attempting to choose means and standard deviations for the randomized variables. The means and standard deviations used, which are intended for demonstration purposes only, are listed in Table I.

TABLE I

Demonstration Means and Standard Deviations

Variable	Mean	Standard Deviation
Repository resaturation time (yr)	100	50
Repository pressure (MPa)	11.3	3.0
K	1.0	0.5
PH	8.0	2.5
PO ₂ (ppm)	5.7	1.5
Density (g/cm ³)		
Dry packing	1.7	0.5
Wet packing	1.5	0.5

The mean repository hydrostatic pressure was chosen to be 11.3 MPa, which is the value used by Westinghouse.⁵ Hydrostatic pressure data was not surveyed to determine the standard deviation, and instead a value of approximately 25 percent of the mean was used. Available data on corrosion exhibit an extremely large standard deviation. However, for demonstration purposes, a standard deviation of 50 percent of the mean was used. The densities of dry and wet packing and the standard deviations for these quantities were based on a survey of packing density requirements for restricting hydrostatic flow in the saturated packing to diffusion.⁵

Figure 1 shows the predicted cumulative probability of container failure that was obtained for the 1982 reference CHLW waste package in basalt with a sample size of 500. The probability that an average container will last 1000 yr is about 50

percent. However, this figure is intended solely to demonstrate the methodology. Considerable model refinement and extensive data review are needed before such a prediction can be regarded with confidence.

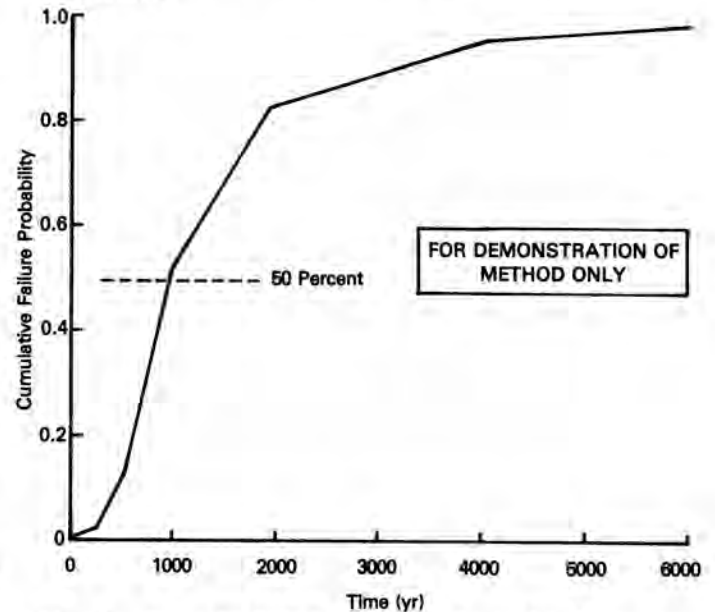


Fig. 1. Demonstration Probability Curve for Container Failure Using WAPPA Code with Modifications and Westinghouse⁵ CHLW Conceptual Waste Package Design for Basalt Repository (500 samples).

A second run was made with identical input but with a different seed for the random number generator, which generates a different set of randomized input parameters. The second predicted cumulative probability was within 2 percent of the first at all years in which the failure probability was calculated. Consequently, the sample size was regarded as adequate for the demonstration. Twenty time steps were used in the WAPPA calculation; thus, in a run of 500 samples, the thermal, stress, and corrosion calculations were repeated almost 10,000 times (requiring a 4-min execution time on an IBM 370 computer).

MODULAR SIMULATION

General Features

Because the barrier system has various layers, a natural assumption would be that the system can be approximated by treating it as several independent components (barriers) operating in standby. This results in a decoupling or modularization of the components. Such a system is well known in reliability analysis⁹ and, if the reliability of each component is known or calculable, results in a particularly simple analytical approach to system reliability. For the radionuclide waste package in particular, the output pdf for the estimated failure time can be written in the form of a multiple convolution integral.¹⁰ This integral is a general formulation that requires only that the failure probability densities for each barrier be available as input. Developing these individual probability densities is not simple, however, and may require computer simulation or other methods that evaluate and combine the various processes that go into causing failure in each barrier. The approximation in this approach assumes there are no process

interactions among the various components; however, this assumption is known to be incorrect in the absolute sense, because the overall environment changes with time, and some processes are affected by the nature of material (e.g., groundwater) passed from one barrier to the next. Therefore, in using this approach, it must be shown either that the interactions are small or that they can be dealt with appropriately.

If the simplifications that lead to modularization are found to be an acceptable approximation to a more general global model, then the number of simulations (computer runs) can be reduced substantially. In a global simulation in which M uncertain parameters are involved and N values of each parameter are to be selected randomly, a total of N^M simulations would be required in the general case. If the M parameters associated with all the barriers are divided equally among four components (barriers) and the same number N of parameter values are chosen, the total number of simulations would be $4(N)^{M/4}$ (four barriers times $N^{M/4}$ simulations per barrier). This oversimplifies the true situation, because it is unlikely that the uncertain parameters would be equally divided. Also, there may be parameters that are common to several components (e.g., temperature-controlling parameters) that would have to be added, thus increasing the value of the exponent.

The physical nature of the barrier system, if exploited judiciously in the modular modeling approach, can reduce greatly the calculations and maintain a high degree of realism and comprehensiveness in the reliability assessment model. Each module can be treated separately to yield a failure pdf. Using precalculated pdf's is a valuable procedure, because the analyst does not have to recalculate all parts of a model if only one part changes. The result is a significant degree of modularity in the reliability assessment model without a significant loss of generality. Combining individual barrier failure pdf's into a system level failure pdf using convolution is discussed in the following section.

Convolution

The concentric barriers of a nuclear waste package are considered a sequential system under reliability theory.¹¹ Each barrier is equivalent to a system component, and only one component functions (or operates) at a time with the others waiting in standby mode. If one operating component of the sequential system fails, one standby component then becomes functional. With concentric barriers, the outermost barrier is the first active component; the inner barriers are in standby mode. During standby time, inner barriers can fail as a result of some internal process (i.e., some standby failure mechanism). If the outer barrier fails, the next inner barrier becomes operational if it has not previously failed. In this case, "operational" means the barrier is subject to attack by processes that increase its failure probability far above that during standby mode.

Time for standby failure modes begins at repository closure; time for active modes begins only after all protective barriers have been breached. Thus, if there is a protection-induced time delay in the onset of a failure mode process, then that process contributes to the probabilities associated with active status. If the failure

process timing is independent of the status of outer barriers, then the process contributes to standby failure probabilities.

Consider a generic standby system consisting of only two barriers: Barrier 1 is the outer barrier, Barrier 2 is the inner barrier. Because both barriers must fail in order for the system to fail, the system failure probability, $f_{12}(t)$, must be less than or equal to the failure probability of the outer barrier, due to the benefit obtained from the inner barrier. However, the failure probability of the second barrier depends on the time of failure of the first. It is necessary to consider every possible failure time, t' , of the first barrier. If Barrier 1 fails at arbitrary time, t' , then the failure probability of the system at a future time, t , hinges on the failure probability of the second barrier for a time period of $t-t'$ while in active mode.

Defining f_2 as the failure probability of the second barrier in the active mode, the probability of its failure at a time $t-t'$ after becoming active is $f_2(t-t')$. The second barrier must also have survived the first period t' while in standby. The corresponding probability would be $R_{2s}(t')$, where R_{2s} is the standby reliability of that barrier, which is defined as one minus the cumulative failure probability. The joint probability of all three events (Barrier 1 fails at t' , Barrier 2 survives in standby for time t' , and Barrier 2 fails in the active mode at time $t-t'$) is $f_1(t')R_{2s}(t')f_2(t-t')$, where $f_1(t')$ is the failure probability of Barrier 1 at time t' . Barrier 1 could fail at any t' from 0 to t ; thus, the probability of system failure in this manner is

$$f_{12}(t) = \int_0^t f_1(t') R_{2s}(t') f_2(t-t') dt' \quad (2)$$

This is recognized as a convolution relationship, i.e., it has the form

$$\int_0^t f_1(t') f_2(t-t') dt' \quad (3)$$

There is also the possibility of system failure because of the failure of Barrier 1 in the active mode at time t and the failure of Barrier 2 in the standby mode at any time t' from 0 to t . Thus, the total failure probability for the two-barrier system is

$$f_{12}(t) = f_1(t) \int_0^t f_{2s}(t') dt' + \int_0^t f_1(t') R_{2s}(t') f_2(t-t') dt' \quad (4)$$

An expression for the failure probability of a three-barrier system is easy to develop if the system is visualized in terms of a two-barrier system with a convolution expression accounting for the extra reliability provided by the third barrier:

$$f_{123}(t) = f_{12}(t) \int_0^t f_{3s}(t') dt' + \int_0^t f_{12}(t') R_{3s}(t') f_3(t-t') dt' \quad (5)$$

The failure probability for any number of components can be computed by applying the convolution relationship recursively if the individual barrier failure probabilities are known.

Example of Modular Simulation

As an example of a modular simulation, a simplified two-barrier waste package model was assembled. The model was intended to be applicable to the basalt repository conceptual waste package, and the modeling approach was similar in some respects to that used in the BWIP Draft Environmental Assessment.⁷ As in that document, borehole wall resaturation and packing infiltration were assumed to occur immediately after closure, and the container was considered to be the first barrier. To simplify the calculations, no attempt was made to determine the failure pdf for the container using physical process models. Instead, the hazard rate for the container due to corrosion failure was assumed to increase linearly with time. The use of time-dependent hazard rates to obtain failure pdf's was suggested previously by Chang and Cho.¹²

The hazard rate, $\lambda(t)$, differs from the failure pdf in that it refers to the current population rather than the original population. It is related to the failure pdf and reliability, R , by the expression¹³

$$\lambda(t) = f(t)/R(t) \quad (6)$$

The assumption of a linear hazard rate results in a failure pdf for the container which is known as the Rayleigh distribution. The Rayleigh distribution is a one parameter distribution of the form

$$f(t) = \lambda t \exp \left[-\lambda t^2/2 \right] \quad (7)$$

$$\mu = \sqrt{\pi/(2\lambda)} \quad (8)$$

$$\sigma^2 = 2/\lambda - \pi/(2\lambda) \quad (9)$$

$$t_p = 1/\sqrt{\lambda} \quad (10)$$

where μ = mean failure time,

σ^2 = variance, and

t_p = peak failure time.

The linear hazard rate was assumed for simplicity and also because it results in a reasonably realistic pdf with a mean value about 1.25 times the peak and a standard deviation of about half the mean. No attempt was made to predict the failure time of the container. Instead, the peak failure time was arbitrarily chosen to be 1000 yr, and this value was used in Eq. (10) to determine the associated container hazard rate. Also, the standby failure probability of the container was assumed to be negligible.

Following the BWIP Draft Environmental Assessment,⁷ the spent fuel cladding was not considered to be a barrier, and the solubility limit of all radionuclides in the groundwater was assumed to be reached immediately after container failure. Consequently, the packing was considered to be the second and final barrier to radionuclide release. In this approach, packing failure is considered to be a binary process (i.e., the radionuclide either has or

has not penetrated), whereas in reality, the release rate is time dependent. However, the maximum release rate is reached shortly after radionuclides first penetrate through the packing, and the time and rate of maximum release are of key interest in the application of regulatory criteria. Consequently, it is reasonable to consider packing failure to be the time of maximum release (t_{max}). Using the one dimensional model of Relyea and Wood¹⁴

$$t_{max} = 0.45 L^2/D'_1 \quad (11)$$

where L = packing thickness (cm),

D'_1 = $D_1/(1 + \rho_1 K_d/\phi_1)$ = retarded diffusion coefficient of packing (cm^2/s),

D_1 = packing diffusion coefficient (cm^2/s),

ρ_1 = packing density (g/cm^3),

K_d = packing radionuclide retention coefficient (cm^3/g), and

ϕ_1 = packing porosity.

The value of t_{max} obtained from Eq. (12) can thus be assumed to be the peak packing failure time, and the associated hazard rate can be computed using Eq. (10). The associated pdf (Eq. (7)) represents the uncertainty in the transport time through the packing due to the uncertainty in packing thickness, retention coefficient, density, and porosity. The standby failure probability of the packing was also assumed to be negligible.

A computer program was written to compute the container and packing hazard rates, failure pdf's, and system failure probability for this simplified two-barrier waste package model. The convolution integral (Eq. (4)) for the system failure probability was numerically evaluated in the program using Simpson's rule. Cumulative system failure probabilities were also computed, and these are illustrated in Fig. 2 for plutonium-240 and carbon-14. The input parameters were those used in the BWIP Draft Environmental Assessment⁷ and are listed below:

K_d = 0 for carbon-14 and 21 for plutonium-240,

L = 19.3 cm,

D_1 = $1 \times 10^{-6} cm^2/s$,

ϕ_1 = 0.3, and

ρ_1 = 1.8 g/cm^3 .

For both cases, the container peak failure time was taken to be 1000 yr, which corresponds to a mean failure time of 1250 yr. However, the cumulative

failure probability for plutonium-240 reaches 0.5 about 800 yr later than for carbon-14. This occurs because the packing failure time, t_{max} , computed using Eq. (11) is only 5.4 yr for carbon-14, but is almost 700 yr for plutonium-240 due to its large retention coefficient.

Limitations of the Convolution Approach

One of the assumptions of the convolution equation is the time invariance of the barrier failure probabilities. If the failure probability of a barrier in the active mode is the same no matter when it is exposed, then it would be time-invariant. For example, if the container has a mean time to failure of 500 yr, it is assumed that it will take an average of 500 yr to fail after groundwater reaches it, regardless of when this occurs.

Obviously, true time-invariance would not hold for chemical attack on barriers because the reactions would proceed faster during higher temperature years shortly after emplacement of the waste than in later, cooler times. Thus, a barrier with a mean time to failure of 500 yr, if exposed to water when the temperature was high, might have an average failure time of 600 yr if it were not exposed until after the repository had cooled.

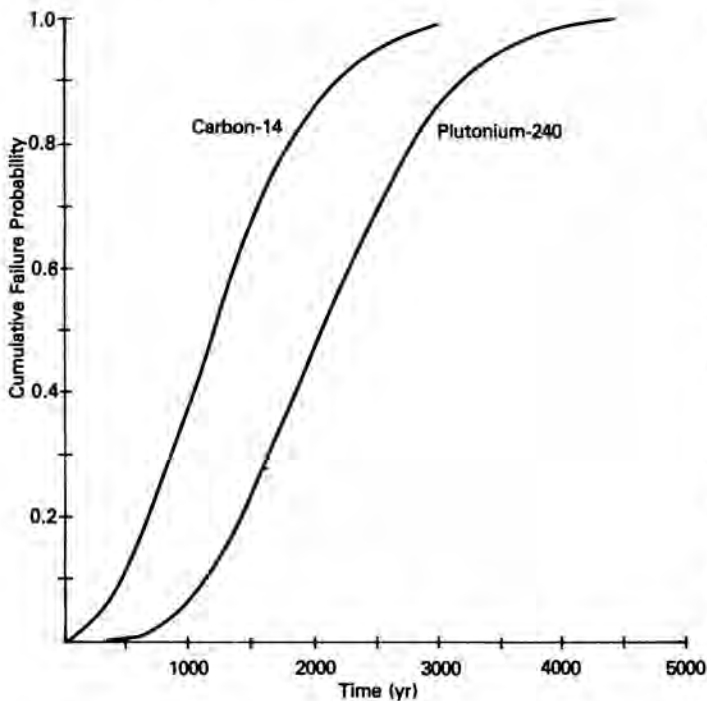


Fig. 2. Example of Waste Package Cumulative Failure Probabilities Computed Using Modular Simulation.

How well the convolution equation works for failure probabilities that are not invariant has not been demonstrated. It may or may not be a good approximation, depending on the barrier process models and their sensitivity to start time. However, the effect of process start time may not be significant compared to the uncertainty in the other parameters. Plans for testing the convolution approach are discussed in "Future Work."

There is always some degree of correlation between degradation processes, even for separate barriers, because of common environmental conditions. If these correlations prove to be significant, then alternative approaches must be considered. Such approaches involve time-dependent, quasi-independent processes. As the process models are used to generate a barrier failure probability, it may be found that this probability is sensitive to start time. For example, if corrosion rates are quite high in the early years of the repository because of high temperature, and if the expected life of the barrier suffering corrosion attack is relatively short so that the early corrosion produces a significant effect on its total life, then the barrier failure probability would be sensitive to start time. This means that the output pdf representing the failure times of a barrier would be conditional on the input pdf used to represent the start time for its degradation processes. The convolution equations assume that barrier failure pdf's are not conditional but are invariant with start time.

There are two ways to deal with this contingency, depending on the degree of the dependence. If the effect of start time is not too severe, then an "average" pdf is developed by running the process models in simulation experiments using uniformly distributed start times. The pdf's thus determined for each barrier would then be used in the convolution equation as usual, and all the efficiencies derived from the modular approach would still be available.

If the output pdf's are considered to be quite sensitive to start time, then the safest procedure would be to use the output failure time pdf for an outer barrier as the input start time pdf for the adjacent inner barrier. Because the output of one barrier model would be used as the input to the next, this method can be termed a cascade approach. Modularity could be preserved, because each barrier would still be modeled separately and no a priori assumptions would be required about the start times (except for the outermost barrier). The convolution equation would not be used in this case; the system failure pdf would be computed directly in the last step as the failure pdf of the last barrier.

However, there are some potential operational difficulties involved in the cascade approach. Each barrier model can be used to produce a pdf only after all prior (outer) barrier pdf's are developed. If an equation or parameter must change in one of the barrier models, then because of the cascading of output pdf's, the entire simulation exercise for all subsequent barriers must be rerun.

RELEASE RATE CALCULATIONS

Radionuclide release rates are needed for several purposes: comparison with the 10 CFR 60 restriction¹ on fractional release rates, for comparison with the 40 CFR 191 restriction² on cumulative releases, and input to subsequent analysis of radionuclide transport in far-field geologic media. Each of the requirements implies a need for an estimate of expected release rate versus time. Estimates of error probabilities for these rates will also be needed.

Computation of the quantity of radionuclides released as a function of time is more complex than computation of waste package failure times discussed in the previous sections. Calculations become three-dimensional, relating probability to radionuclide release rate and time in contrast to the two-dimensional probability versus failure time curve. Because each radionuclide is likely to have a different release rate, the generation of this three-dimensional probability surface is needed for each important radionuclide present.

One method is to develop nominal curves describing fractional release rates since the occurrence of waste package failure. A series of simulation runs would be required to produce an ensemble of release rate curves corresponding to randomly selected parameter values. The nominal curve, representing the expected fractional release rate, would be found from this data using regression analysis. The uncertainty associated with that curve would be characterized by an empirical probability distribution that could easily be computed from the same simulation output. This approach assumes that there is no direct interaction between the fraction release rate curve and the time at which failure of the last protective barrier occurs.

The nominal release rate curve and its associated probability distribution can be combined with the probability distribution for each container failure time using convolution. This results in a three-dimensional surface relating probability to release rate and to time since repository closure. This is probably a good approximation to the problem when the barriers have long lifetimes and temperature is no longer a factor. It is essentially the approach used by BWIP in their Draft Environmental Assessment.⁷

A second method would be to couple the waste package failure distribution and the radionuclide release rate in a combined simulation run. Each simulation run would sample the waste package failure time and other uncertain parameters before beginning the calculations of radionuclide transport through the packing. This is a more accurate approach because it keeps the release rate calculations closely coupled with the release start time calculations. They would be based on a common sampling of random environmental parameters. Assumptions associated with decoupling release start time from subsequent release rates would not be necessary, and the use of convolution for recombining the two would not be needed. However, this closely coupled approach would require more computer time than the more modular approach using convolution.

FUTURE WORK

Work has begun to examine the validity and limitations of modular simulation in comparison to global simulation and other methods such as cascaded approaches. At this stage, the effort is limited to examining the comparable validity of alternative approaches. The intent is not to provide meaningful predictions of repository performance, because although the available process models and empirical data will be used, these models and data may not have been subjected to critical review and analysis. In an analysis of alternatives, the main requirement is that the model and data be sufficiently similar to permit a comparison. Issues of absolute validity can be postponed for future review. The principal question currently is the extent and importance of

interactions among processes involving different barriers and their effects on waste package performance assessment methodology.

Future work will also include the addition of standby failure modes and an examination of the effects of initial flaws and low probability external events such as earthquakes and human intrusion.

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