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"SUBSTANTIALLY COMPLETE CONTAINMENT" – EXAMPLE ANALYSIS OF A REFERENCE CONTAINER

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Prepared by

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PREVIOUS REPORTS IN SERIES

Number	Name	Date Issued
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NUREG/CR-5639	Uncertainty Evaluation Methods for Waste Package Performance Assessment	January 1991
CNWRA 90-007	"Substantially Complete Containment" Feasibility Assessment and Alternatives Report	September 1990
CNWRA 92-016	"Substantially Complete Containment" (SCC) Elicitation Report	August 1992
Letter Report	Selection and Evaluation of Models for Substantially Complete Containment Example Problem	September 1992

ABSTRACT

This report represents the analyses and results of an example problem conducted in support of evaluating the "substantially complete containment" rule for waste packages in 10 CFR Part 60. The waste package in this example problem is represented by a thin-walled metallic container emplaced in a vertical borehole. A computer code, Substantially Complete Containment EXample (SCCEX), currently under development, was adopted to perform the deterministic parts of the calculations for a single container. Several models representing the repository thermal fields, near-field environment, corrosion of container materials, including localized corrosion and stress corrosion cracking, as well as mechanical failures were coupled to calculate the time-to-wetting and the time-to-failure of waste packages for an unsaturated repository site. A probabilistic method was adapted to generate cumulative distribution functions (CDFs) for failures of multiple waste packages arranged in a simulated square repository. For evaluating the various corrosion processes, the corrosion potential is used as a key parameter in conjunction with critical potentials for localized corrosion. This concept is shown to be a generally powerful approach for evaluating waste package lifetimes in a geologic repository. The report also presents the assumptions incorporated to simplify the models and the various limitations of the calculations performed in the example problem.

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The CNWRA-generated original data contained in this report meets quality assurance requirements described in the CNWRA Quality Assurance Manual. Sources for other data should be consulted for determining the level of quality for those data.

SCCEX and SMLEXC computer codes were used for analyses contained in this report. These computer codes are not controlled under the CNWRA's Software Configuration Procedures, and this report describes the development of these computer codes, however, the codes have not been sufficiently developed to be placed under the CNWRA Configuration Management system.

1 INTRODUCTION

The words "substantially complete containment" (SCC) in the subsystem performance requirements for the waste package, as described in 10 CFR 60.113, have led to several interpretations about the implications in meeting such a regulation. This has resulted in identifying that the rule has a regulatory uncertainty (CNWRA 90-003). The U.S. Nuclear Regulatory Commission (NRC), in an approach to resolve the SCC issue, has contracted with the Center for Nuclear Waste Regulatory Analyses (CNWRA) to conduct a sequence of technical activities to enhance the bases for further guidance to the licensee on this subject. The earlier focus for the technical activities was to determine if a quantitative criteria for SCC was feasible. The CNWRA developed four reports that addressed the necessary technical considerations for SCC, evaluated methods to characterize uncertainties, proposed a framework based on probabilistic methods for a rule or criterion including options for regulatory presentations, and conducted a survey of preference among the options from a selected number of the NRC staff. After the completion of these activities, the NRC further directed the CNWRA to develop and provide calculated results for an example problem for containment by waste packages, and prepare an informational report on the field experience of underground and other engineered structures. The purpose of this report is to present the SCC example problem and the calculated results of a number of analyses.

Unlike conventional engineering applications, the time scales for the required waste package performance are significantly longer, and the documented long-term experience on existing engineering structures is very limited or nonexistent. The required performance for a waste package in 10 CFR 60.113 is based on anticipated processes and events. This will enable a designer to develop a waste package based on a set of defined or expected conditions. However, a problem arises when the long-term environmental and controlling near-field processes have to be defined. Toward attempting to define the applicable processes and conditions, a significant effort is underway by the U.S. Department of Energy (DOE) to characterize the potential repository site at Yucca Mountain. In postulating future states (i.e., disruptive scenarios) at any repository site, there is bound to be residual uncertainty in various conditions that cannot be fully determined. Hence, sufficient margins of safety should be developed and incorporated into the designs. In developing an example problem, several key assumptions have to be made. The assumptions and the determination of the anticipated process and events for the problem analyzed in this report are based on CNWRA staff judgments and current information available from the literature.

The waste package design concept used in the example problem is the reference design presented in the Site Characterization Plan (SCP) (U.S. Department of Energy, 1988a). Here, the waste package consists of a relatively thin-walled, corrosion-resistant metal container placed in an oversized vertical borehole in the repository. The geometry has been simplified to permit the use of simple analytical expressions for the application of the various mechanical models used in the problem. The container materials conform generally to the austenitic alloys described in the SCP. However, there are significant departures in the assumptions on the chemical and loading environments from that described in the SCP.

The modeling of the near-field environment for the example problem is focused on the time dependent evolution of the chemical environment on the waste package surface. This is particularly important in the case of an unsaturated site, where the potential exists for groundwater to drip on a thermally hot waste package and subsequently, on evaporation, deposit salts on the waste package surface. The concentration of salts in the presence of future groundwater intrusion can promote and accelerate the corrosion of certain waste package materials. Associated with models that describe the slow degradation processes of metal containers are models that represent waste package behavior under high magnitude single or multiple load events. Collectively, these models describe when and how a given waste package is predicted to fail. A set of models was selected for the example problem to represent the important failure mechanisms for the chosen design concept and predicted environments. Due to the simplified nature of the models and the assumptions and approximations made, these models do not necessarily provide a quantitative representation of the actual conditions that may be present in an unsaturated repository site as the one modeled here.

The analyses consist of both a set of deterministic and a set of probabilistic calculations. The calculations are performed through the use of computer codes currently under development at the CNWRA. The deterministic calculations are performed by the Substantially Complete Containment EXample (SCCEX) problem code, while the probabilistic calculation is performed by the executive driver program named SMLEXC. SMLEXC is a modified version of a system code used in the Iterative Performance Assessment (IPA) project at the CNWRA. The results of the deterministic calculations are evaluated for various parameters and the probabilistic calculations are represented as cumulative distribution functions (CDFs) and probability functions (PDFs) for failure of a number of waste packages.

The calculations presented in this report are primarily intended to demonstrate an approach for evaluating containment by a waste package and point to areas requiring more detailed analysis. It is not intended, in this report, to demonstrate the suitability or unsuitability of any given waste package material or design in terms of performance requirements. For the purposes of simplicity, the failure of a waste package in this analysis is defined as the condition of the waste package when the container walls are penetrated by localized corrosion or by stress corrosion cracking. Failure can also occur by mechanically dominated processes. The following sections of the report address the details of the example problem, the results obtained, and a discussion of the results.

2 CALCULATIONAL METHODOLOGY FOR THE SCC EXAMPLE PROBLEM

The assessment of containment of high-level waste (HLW) in a waste package involves the use of several computational models that are interconnected both spatially and temporally in a geologic repository. To conduct such an assessment, a computer code currently under development has been applied to the example problem of a reference container. In the SCCEX code, a methodology is established for making deterministic predictions of waste package performance in a repository environment. In implementing the current development of the SCCEX code, several simplifying assumptions were made to both the models and the calculational algorithms.

The waste package for the example problem is represented by a thin-walled metallic container placed in an oversized vertical borehole. The geometry and materials used are generally consistent with the reference design presented in the SCP (U.S. Department of Energy, 1988b). An important aspect of determining the failure of a waste package to contain the waste is the definition of the term failure. For the analyses performed here, it is assumed that the waste package fails when a through-wall penetration develops in the container as a result of localized corrosion or stress corrosion cracking. Alternatively, it is postulated that failure may also occur by mechanical fracture, by yield failure, or following a sufficient reduction of wall thickness by general or localized corrosion, as a result of buckling.

In the evaluation of containment, it should be recognized that the waste packages could be exposed to varying environmental conditions. This implies that the calculations should also account for these variabilities. Also, there are uncertainties in the parameters used in various models. In the example problem, the uncertainty in parameter values is addressed by adopting a probabilistic analysis method.

This section presents the computer code, the numerical approach, and the description of the models dealing with the waste package environment, corrosion processes, and mechanical failure conditions for the example problem. The calculations using the SCCEX code represent the deterministic analysis for a single waste package for various parameters of interest. The description of the code is included in Appendix A. The probability of failure of multiple waste packages is calculated using the executive driver module named SMLEXC. The SCCEX code operates under the SMLEXC code structure for the probabilistic analyses.

2.1 SINGLE WASTE PACKAGE CALCULATIONS USING SCCEX CODE

The SCCEX code example flow diagram is presented in Figure 2-1. The input data required to execute the SCCEX code for this problem include the following: (i) total simulation time, (ii) geometry of container, (iii) temperature parameters, (iv) evaporation parameters, (v) solver selection and related parameters, and (vi) corrosion parameters. The input and output structure for the SCCEX code is discussed in detail in Appendix B. The idealized repository is assumed to be a square area with an assumed one-eighth symmetry for the temperature field containing equally spaced waste packages. Based on the symmetry, the SCCEX code divides the repository into calculation cells. A typical cell structure for the repository is shown in Figure 2-2. For the example problem, the calculation cells on the diagonal occur four times in the repository is called the weighting factor which is used to calculate the total number of failures in the repository.



Figure 2-1. Flow diagram of the SCCEX code



Note: A = 4 cells, B = 8 cells, modeled as 1/8 symmetry

Figure 2-2. Definition of repository cells and groups

For each cell, the calculations begin with an estimate of thermal loading and resulting temperature effects. The average repository temperature, the container surface temperature, and the container internal temperature are calculated as a function of time and stored in arrays. In a later section of the code, the thermal calculations are combined with water drip rates to estimate the amount of water on the container surface and its composition.

Based on the calculated water composition and temperature, either general corrosion, pit/crevice corrosion, or stress corrosion cracking may take place and the corresponding corrosion rate are estimated. The container temperature, corrosion penetration depth, and area penetrated by corrosion are then used to assess the structural integrity of the container. A deterministic seismic induced stress is assumed and compared with the residual strengths of buckling, fracture, and yield to determine whether a mechanical failure occurs or not. The above process is iterated until the end simulation time has been reached. Selected calculational results such as the time-to-wetting and time-to-failure are stored in files.

2.2 MULTIPLE WASTE PACKAGE CALCULATIONS USING SMILEXC CODE

SMLEXC, as shown in Figure 2-3, contains four basic parts: (i) the executive, (ii) algorithm to sample from statistical distributions, (iii) preprocessor for the SCCEX code input, and (iv) SCCEX code to compute the time-to-wetting and the time-to-failure. The SMLEXC executive code directs data flow between different parts and controls their execution. Figure 2-3 shows schematically the data flow and execution dependencies of the parts of the SMLEXC system. To start the SMLEXC executive code, a SMLEXC input file, smlexc.inp (see Appendix C for more discussions), which defines total number of simulation vectors and all executable file names and addresses for other parts, is required.

The algorithm used to sample from statistical distributions is called the Latin Hypercube Sampling (LHS) method. The sampling method in the LHS ensures that all parameter vectors in a set are equally probable. Thus, if N vectors are included in a set, then each vector has a probability of occurrence of 1/N. Simulations are performed with each vector in turn, resulting in the calculations of N event times. It is obvious that each event time is equiprobable with a probability of 1/N. To run this algorithm, a statistical input file, smllhs.dat (see Appendix C for more discussions), which summarizes statistical distribution types and bounds of all random properties, is required.

Based on the sampled data using the LHS, a preprocessor code was developed to map these sampled data into a valid SCCEX input deck. Next, this SCCEX input deck is used to compute the time-to-wetting and the time-to-failure for each calculation cell. The same process is iterated until the total number of calculation cells has been reached. The time-to-failure and time-to-wetting results for all calculation cells and vectors are stored in both SMLEXC executive code and a data file, postdd.dat. For data stored in SMLEXC, each time event data (e.g., time-to-failure) will be sorted and an empirical CDF will be calculated according to each calculation cell's weight factor. This approach produces the failure (or wetting) percentage, however, it neglects the most important information such as the critical location of the cell. To overcome this disadvantage, the data file, postdd.dat, is analyzed by using a probabilistic postprocessor code (Appendix D) to construct necessary CDFs and PDFs for the worst cells and cumulative number of failures.



Figure 2-3. Diagram showing the data flow and the execution dependencies of the SMLEXC system and the input/output file names

2.3 DESCRIPTION OF MODELS

This section is a brief description of the various models within the code structure along with the type of inputs and outputs. More detailed rationale, descriptions, and limitations of the various models can be found in the Engineered Barrier System Performance Assessment Codes (EBSPAC) progress report (Sridhar et al., 1993).

2.3.1 Thermal Model

This is a simplified model that considers conduction as the only heat-transfer mechanism. The repository is considered to be a volumetric source with a square shape having a uniform and constant thermal conductivity and heat capacity. For a rectangular repository, the temperature field for a homogeneous, isotropic, and an infinite three-dimensional medium is given in terms of the Green's functions as shown below:

$$G = \frac{(G_x G_y G_z)}{8 \rho C_p w^2 h}$$
(2-1)

$$G_{x} = \operatorname{Erf}\left(\frac{\frac{w}{2}+x}{\sqrt{4\alpha t}}\right) + \operatorname{Erf}\left(\frac{\frac{w}{2}-x}{\sqrt{4\alpha t}}\right)$$

$$G_{y} = \operatorname{Erf}\left(\frac{\frac{w}{2}+y}{\sqrt{4\alpha t}}\right) + \operatorname{Erf}\left(\frac{\frac{w}{2}-y}{\sqrt{4\alpha t}}\right)$$

$$G_{z} = \operatorname{Erf}\left(\frac{\frac{h}{2}+z}{\sqrt{4\alpha t}}\right) + \operatorname{Erf}\left(\frac{\frac{h}{2}-z}{\sqrt{4\alpha t}}\right)$$
(2-2)

where

 $\rho C_p = \text{density times heat capacity}$ w = width of square repository h = height of repository x,y,z = distance from center of repository (assumed zero) $\alpha = \kappa/\rho C_p = \text{thermal diffusivity}$ $\kappa = \text{thermal conductivity}$

The time and spatially dependent temperature is obtained from a convolution integral with the heat generation rate

$$T(x,y,z,t) = \begin{bmatrix} t \\ \int \\ 0 \end{bmatrix} Q(\tau) m G(t - \tau) d\tau + T_{ref}$$
(2-3)

where

t = time Q = heat generation rate per kg initial heavy metal m = amount of heavy metal $T_{ref} = initial temperature (23 °C)$

The rate of heat generation data for heat generation (Q) is based upon data reported in U.S. Department of Energy (1993) and described in Section 3.1. In addition to the overall heating of the repository, the temperature difference between the surface of the waste package and the rock some distance away is modeled using a steady-state, heat conduction model for a radial geometry. The steady-state assumption, in contrast to the time-dependent variation of the overall repository temperature [Eq. (2-3)], is used because the overall repository temperature decreases much more slowly as a result of the radioactive decay than local (waste package scale) temperature changes due to conduction over relatively short distances. The steady-state temperature difference between the surface of a container and the rock some distance away is given by

$$\Delta T = \frac{mQ}{2\pi l} \left[\frac{\ln\left(\frac{r_2}{r_1}\right)}{\kappa_p} + \frac{\ln\left(\frac{r_3}{r_2}\right)}{\kappa_r} \right]$$
(2-4)

where

- r_1, r_2, r_3 = radial distance of container wall, packing/rock interface, and outer boundary respectively from container centerline
- κ_p, κ_r = thermal conductivity of rock and packing materials
- = length of container

The output of this model is the temperature distribution in a cartesian coordinate from the centerline of the repository and the temperature drop between an individual container and the surrounding rock at an assumed distance for any given time period. This simplified thermal model was adopted to facilitate the parametric calculations. However, it has limitations arising from the effect of the outer distance, r_3 , on the calculated value of ΔT and the fact that ΔT is assumed to be independent of the spacing between containers. In addition, it can be expected that a temperature gradient develops in the vertical direction. An alternative approach that may be incorporated in future versions of this code is the use of other thermal codes such as V-TOUGH (Nitao, 1989).

2.3.2 Environment Model

In this model, the evolution of the environment on the waste container surface is computed. The environment around the container is dictated by the rate of evaporation of water contacting the container, the rate of influx of water, the types of salts precipitated, and their effect in reducing the vapor pressure of water on the container surface which promotes movement of water vapor to or away from the container surface. The outputs of this model are the time at which a water film is stabilized on the container (time-to-wetting or wetting time), the thickness of the scale layer precipitated on the container surface, the area covered by a water film on the surface of the container, and the concentration of ionic species in the water film. It is assumed that the water film had a limited thickness, and the wetted area is calculated from the volume of water available at the container surface using an arbitrary value for the thickness of the water film.

The amount of water on the container surface, the amount of scale deposited, the amount of effluent generated, the amount of soluble salts on the container surface, and the depth of penetration by corrosion are calculated by solving a set of ordinary differential equations. The material balance equations are

$$\frac{dV}{dt} = Q_{in} - Q_{out} - \frac{EM_{H_2O}}{\rho_{H_2O}}$$
(2-5)

$$\frac{ds}{dt} = C_{in}^{s} Q_{in} - C_{out}^{s} Q_{out}$$
(2-6)

$$\frac{dS}{dt} = C_{in}^{S}Q_{in} - C_{out}^{S}Q_{out}$$
(2-7)

$$\frac{d\Gamma}{dt} = Q_{out} \tag{2-8}$$

$$\frac{dL}{dt} = r \tag{2-9}$$

where

V = volume of water on waste container surface $Q_{in}, Q_{out} = volumetric flow rate of water onto and exiting the waste container surface$ E = molar evaporation rate from the entire container surface without end effects $M_{H_2O} = molecular weight of water$ $\rho_{H_2O} = density of water$ S = mass of soluble salts on container surface

S	-	mass of scale forming compounds on container surface			
C _{in} , C _{out}	=	input and output aqueous concentration of soluble salts or scale-forming			
		compounds			
Г	=	cumulative amount of effluent water			
L	=	depth of penetration by corrosion			
r	=	corrosion rate, either passive or active			

When the container is completely covered with water, the steady state conditions correspond to dV/dt = 0, and Q_{out} is the difference between Q_{in} and the evaporation rate.

Liquid water can reach the container surface by several mechanisms including matrix flow, fracture flow, and/or condensate dripping. Flow of water on the container is not calculated in the SCCEX code, but it can be specified by two different options. The first option is to directly input the Darcy velocity near the container as a function of time in tabular format. The flow onto the container surface is then the input flow rate times the representative area of the individual waste package times an input factor specifying the proportion of water passing a waste package that actually drips onto the container surface.

The second option is more complex and assumes a larger scenario. The imagined scenario is the drying of the repository by the thermal loading. The drying leads to upward movement of some water with shedding of water around the sides of the heated area. The concept has been assumed to be a hydrothermal umbrella protecting the repository. The hydrothermal umbrella tends to protect the portions of the repository heated above the boiling point of water from water dripping onto the containers. As a result of the umbrella, the flux of water onto the repository is diverted around the center of the repository to the outer edges where temperatures are below the boiling point of water. Further out from the edge of the umbrella, the downward flux of water reverts to the input (background) flow rate. This scenario is implemented in the code relative to an input temperature specified at the edge of the umbrella along with a positive or negative variation within a range. The physical thickness of the umbrella edge (where enhanced flow occurs) and the surface area of impingment are also inputs to the code. When the temperature of the rock near the container surface is in the range of the umbrella edge, then the downward flux of water impinging on the umbrella is diverted to the outer edge of the umbrella. The calculation is simplified by assuming the hydrothermal umbrella is circular in shape. Additionally, it is assumed that most of the initial pore waters are diverted around the repository during the initial thermal period. Outside the edge of the umbrella, the input flux of water hits the container surface as described in Option 1.

In both of the options, an initial impingement of water can be implicitly applied at zero time. The physical basis for this initial impingement of water comes from two separate scenarios. Experimental tests have indicated that wetting of the container surface is possible during the initial heating of the rock surrounding a heated container. Water will tend to evaporate from the container almost instantaneously (relative to the long periods of interest) leaving behind soluble salts and precipitated minerals (scale) on the container surface. For this reason, the initial amount of water is specified in terms of soluble salt mass and scale mass, rather than as a volume of water. The second source of the initial amount of water is dripping from soluble salt deposits near the container. When the water is evaporated from the rocks near the container, deposits of soluble salts may be left behind, especially at high evaporation sites such as fracture walls. As the repository cools, the soluble salt deposits can pick up moisture related to osmotic lowering of vapor pressure by dissolved ions. It is assumed that some portion of the condensed, osmotic water may drip onto the container surface. Because the container surface is always hotter than the surrounding rocks, such dripping would occur only prior to the time at which water can be held osmotically on the container surface. For this reason, the actual time of dripping is not important and the calculations are simplified through specification of an initial amount of soluble salt on the container surface.

The evaporation rate of water around the waste package is driven by the difference in temperature between the waste package and the rock a few meters away, where liquid water is present in the pores and the relative humidity is close to one. When water reaches the container surface by any of the processes discussed previously, the temperature of the water is raised. The increase in temperature of the water on the container surface causes the vapor pressure to be elevated relative to that of the water present outside of the dry-out zone. The vapor pressure difference promotes evaporation of the water from the container surface. Because of the small amounts of water anticipated and the large mass of the container, the loss of sensible and latent heat by water heating and evaporation from the container surface is insignificant in the overall energy balance. The rate of evaporation is thus limited by mass transport of water vapor across the dry-out zone if the temperature of the system is below the boiling point. When the container temperature exceeds the boiling point, evaporation is effectively instantaneous.

Below the boiling point of the solution, the rate of evaporation is a function of overall temperature and temperature drop between the container and surrounding rock. The flux equation for binary diffusion of water vapor through air assuming infinite permeability of the medium (i.e., constant pressure) is given by Bird et al. (1960).

$$N_{\rm H_2O} = x_{\rm H_2O} (N_{\rm H_2O} + N_{\rm air}) - c D \tau \phi \nabla x_{\rm H_2O}$$
(2-10)

where

N _{H2} O	=	molar flux of water vapor
N _{air}	=	molar flux of air
x _{H2} 0	=	mole fraction of water vapor
c	=	total molar concentration of gas
D	=	binary diffusion coefficient
τ	=	tortuosity factor
φ	=	rock porosity

Solving for steady-state evaporation in a radial geometry gives

$$E = 2\pi lc D\tau \phi \frac{\ln\left(\frac{1-x_1}{1-x_3}\right)}{\ln\left(\frac{r_1}{r_3}\right)}$$
(2-11)

where

$$E$$
 = molar evaporation rate from the entire container surface without end effects
 x_1, x_3 = mole fraction of water vapor at container surface and at distance, respectively

The tortuosity and porosity factors are treated as independent parameters. The air gap zone around the waste container can be ignored because it has greater diffusion rates than the surrounding rocks. The diffusion coefficient in the air/water vapor system in m^2/s is assumed to be given by (Treybal, 1980).

$$D = 3.05 \times 10^{-5} \left(\frac{760}{680}\right) \left(\frac{T}{T_{\rm ref}}\right)^{1.5}$$
(2-12)

where the pressure at the repository horizon is taken as 680 mm Hg, and the reference temperature $(T_{ref}) = 232$ °K (59 °C). The vapor pressure of water as a function of temperature is taken from Perry's Handbook (Perry and Chilton, 1973). Conversions between vapor pressure, concentration, and mole fraction are performed with the ideal gas law. The tortuosity factor is taken from Jury et al. (1991). Jury et al. (1991) discuss mechanisms that may enhance water vapor migration in soil by a factor of two to three times greater than predicted by the above equations, although the theoretical rationale is limited to temperatures of less than 60 °C and high relative humidity.

The time-to-wetting and the concentration of the solution on the container surface are interrelated. Partial evaporation of groundwaters similar to J-13 water has been considered by Garrels and MacKenzie (1966). They conclude that evaporation at equilibrium with the atmosphere results in precipitation of silicate and carbonate minerals, leading to an alkaline brine solution. Evaporation of southern Nevada waters with the geochemical codes PHREEQE and EQ3/6 likewise leads to alkaline brine solutions (Murphy, 1991; Vaniman et al., 1992). As evaporation continues, the remaining aqueous solution becomes more concentrated, and the vapor pressure of the water is decreased. The maximum extent of the vapor pressure decrease depends upon the final composition of the solution prior to complete drying). The composition of water at the evaporation endpoint is currently unknown and may depend upon evaporation rate relative to drip rate, container temperature, vapor composition, presence or absence of rock particles in the solution, and the composition of the dripping water—all of which vary between containers and even along a single container. The solutes present at the evaporation endpoint play a pivotal role in controlling water access to the waste container by lowering the vapor pressure of water.

The amount of water held on the container by solute forces is dependent upon the vapor pressure of water in the repository horizon and the mass of salts present on the container. The amount of salts present is proportional to the volume of water evaporated and the initial composition of the dripping water. As discussed previously, the actual amount of dripping water and the composition of the dripping water are likely to be highly variable in time and space and are difficult to predict with precision. Nonetheless, the overall range expected can be examined with calculations. Assuming that the dripping water has the composition of J-13 well water and the final solution is composed of sodium chloride at 25-weight percent dissolved salt, the solute effects are significant. Assuming the brine film on the container remains at 25-percent dissolved salt by weight, then for each liter of water dripping on the container, the brine film grows by 0.065 ml (0.0065 percent of the water dripping on the waste package remains in the salt film). The water lost can be replenished by diffusion of water vapor towards the waste package. Thus, chemical reactions on or in the waste package that consume water do not lower the amount of water present in the salt film unless the salt itself is consumed in the chemical reactions. Generation of additional salts by chemical reactions on the container or waste (e.g., by wasteform alteration or corrosion), would tend to increase the volume of water on the salt film.

Heat loading, combined with limited water supply, leads to creation of a desiccated zone around the waste package in which the relative humidity is decreased well below one. Three conditions can cause water to be present within this zone: (i) adsorbed or capillary water, (ii) solute-caused lowering in vapor pressure, and (iii) transient water related to fracture drainage. Vapor pressure lowering in capillaries is described with Kelvin's equation.

$$b_{\text{capillary}} = \frac{p_{\text{capillary}}}{p^0} = \exp\left[\frac{\psi Mg}{RT}\right]$$
 (2-13)

Vapor pressure lowering from solutes is a function of concentration and solute composition.

$$b_{\text{solute}} = \left(\frac{p_{\text{solute}}}{p^0}\right) = f(C_1, C_2, \dots, C_i)$$
(2-14)

Total vapor pressure lowering is a combination of solute and capillary effects.

$$\frac{p_{\text{total}}}{p^0} = b_{\text{capillary}} \cdot b_{\text{solute}}$$
(2-15)

where

 p^0 = vapor pressure at temperature for pure water.

If the waste container is surrounded with an air gap or with crushed rock (gravel), then the unsaturated hydraulic conductivity of the packing will be near zero. In this situation, the vapor pressure of water on the surface of the waste container is determined by the vapor pressure of water in the rock near the waste package. At a constant vapor pressure of water, the relative humidity at any point is a function only of temperature (i.e., temperature determines p^0). At any point, water will evaporate or condense until the waste package vapor pressure of water is reached. On the average, temperature will decrease from the centerline of the waste package outward in a radial direction. The salinity or composition of water in this system is then determined by temperature, presence of small pores, and presence of soluble salts. In an idealized, homogeneous, porous medium, water and soluble salts would tend to redistribute towards a state where vapor pressure of water and capillary pressure were both constant. Gradients in vapor pressure of water lead to vapor diffusion, which is very fast at high temperatures and waste package size scales. Gradients in capillary pressure lead to liquid flow, a relatively slow process at high capillary pressure. This liquid flow, combined with the heat-generated circulation, leads to greater salinity towards the waste package centerline.

In the code, the salt that is precipitated is assumed to be sodium chloride. Based on this, the <u>time-to-wetting is calculated</u> by assuming that wetting occurs when the temperature of the container is such that a saturated solution of NaCl can become thermodynamically stable as a liquid film on the container surface at a temperature higher than the boiling temperature of pure water. The vapor pressure of water in the saturated solution on the container surface is then lower than the vapor pressure of pure water at the outer boundary temperature. The assumed chemical composition (i.e., saturated chloride solution) is then used as input to the corrosion model. Future versions of the code will consider the chemistry of the final solution more rigorously because this is a limitation of the current version. Inhibiting species for localized corrosion (i.e., nitrate) as well as other anions, such as sulfate, bicarbonate, etc., need to be considered.

2.3.3 Corrosion Models

The corrosion models calculate the rates of uniform corrosion, localized corrosion, and stress corrosion cracking. The corrosion process at any given time period is dictated by the corrosion potential and the appropriate critical potential for a given corrosion process. The corrosion potential is the natural potential established at the metal/solution interface when a metal is immersed in a given environment. For example, if the corrosion potential exceeds the critical potential for pit initiation, pits are assumed to initiate and grow. If the corrosion potential falls below the repassivation potential, previously growing pits are assumed to cease growing and the material corrodes at a uniform rate through a passive film. The critical potentials are assumed to have a range of values due to the stochastic nature of the localized corrosion. This is justifiable based on literature data (Sridhar et al., 1993) which suggest that these critical potentials for the two localized corrosion processes coincide at temperatures higher than 20 °C. The existence of critical potentials for stress corrosion cracking is less certain. In the example analysis, the critical potential for stress corrosion cracking is assumed to be the repassivation potential for localized corrosion.

2.3.3.1 Corrosion Potential

The corrosion potential is defined as the potential at which the current due to all the cathodic processes is equal to the current due to all the anodic processes including the electrochemical dissolution of the metal, as indicated by

$$\sum_{j=1}^{n} I_{a,j} - \sum_{j=1}^{n} I_{c,j} = 0$$
(2-16)

where $I_{a,j}$ refer to the anodic (oxidation) currents including that of the metal dissolution (called the corrosion current, I_{corr}) and $I_{c,j}$ refer to the cathodic (reduction) currents. If the anodic and cathodic processes occur uniformly throughout the surface of interest, then Eq. (2-16) can be written in terms of appropriate current densities. However, once localized corrosion initiates, this assumption is no longer valid since physical separation of anodic and cathodic areas occurs. The areas of passive corrosion, in which cathodic reactions take place, must be considered separately from the areas of active corrosion. Similarly, if a bimetallic container is used wherein the outer container is assumed to develop through-wall

defects, then the areas of the outer container and the exposed inner container must be considered. In the following sections, uniform distribution of cathodic and anodic areas is assumed for simplicity.

The two cathodic reactions assumed in the present code are the oxygen reduction and hydrogen evolution reactions. The oxygen reduction reaction is assumed to be a mixture of activation controlled charge transfer process and molecular diffusion controlled transport process. The resulting current density can be written as

$$i_{O_2} = -k_{O_2} C_{O_2}^{\text{bulk}} \frac{\exp \left(\frac{z_{O_2} \beta F E_{\text{corr}}}{RT}\right)}{\left[1 + \left(\frac{k_{O_2} \delta \exp \left(-\frac{z_{O_2} \beta F E_{\text{corr}}}{RT}\right)}{4F D_{O_2} \tau \phi}\right)\right]}$$
(2-17)

where

k ₀₂	=	reaction rate constant for the oxygen reduction reaction
E	=	corrosion potential
F	=	Faraday constant
α	=	charge transfer coefficient
R	=	gas constant
Τ	=	temperature in °K
z _{0,}	=	number of electrons involved in the process per mole
D_{0_2}	=	diffusivity of oxygen in aqueous solution
τ	=	tortuosity
φ	=	porosity
δ	=	thickness of the diffusion layer (e.g., scale or water film)
$C_{\mathrm{O}_2}^{\mathrm{bulk}}$	=	bulk concentration of oxygen in solution.

and $\beta = 1 - \alpha$. For the oxygen reduction reaction, the bulk concentration is related to the partial pressure through Henry's law

$$C_{O_2}^{\text{bulk}} = K_H \cdot p_{O_2} \tag{2-18}$$

where P_{O_2} is the partial pressure of oxygen over the solution and K_H is the Henry's law constant for oxygen solubility.

The reaction rate constant is not usually measured directly, but can be calculated from the exchange current density using the following equation

$$i_{O_2}^0 = k_{O_2} C_{O_2}^{\text{bulk}} \exp\left(-\frac{z_{O_2}(1-\alpha)F}{RT}E_{eq}^{O_2}\right)$$
 (2-19)

where

 $i_{O_2}^0$ = exchange current density $E_{eq}^{O_2}$ = equilibrium potential for the oxygen evolution reaction

For the hydrogen evolution reaction or the water reduction reaction, the cathodic current is assumed to be dictated only by the charge transfer process. The cathodic current density is given by

$$i_{\rm H_2O} = -k_{\rm H_2O} \left[\exp\left(-\frac{\beta_{\rm H_2O} z_{\rm H_2O} F}{RT} E_{\rm corr} \right) \right]$$
 (2-20)

where

 $k_{\rm H_2O}$ = reaction rate constant for the water reduction reaction $E_{\rm corr}$ = corrosion potential

The reaction rate constant can be calculated from the appropriate exchange current density for the hydrogen evolution reaction similar to that shown in Eq. (2-19). The equilibrium potential for water reduction/hydrogen evolution will depend on the bulk concentration of the H^+ ion which is related to the pH. The temperature dependence of the reaction rate constants for the oxygen evolution and the water reduction reactions are assumed to be given by an Arrhenius type relationship as shown in Eq. (2-21).

$$k = k_{298 \, \circ_{\rm K}} \, \exp\left[\frac{E_a}{R} \left(\frac{1}{298} - \frac{1}{T}\right)\right]$$
 (2-21)

where E_a is the activation energy for the particular cathodic reaction and $k_{298} \cdot K$ is the reaction rate constant at 298 °K.

The anodic current density is assumed to be equal to the passive current density of the alloy and to be independent of the potential. A survey of the literature on stainless steels also indicated that the passive current density, at least to a first approximation, is independent of temperature up to approximately 100 °C. The corrosion potential is then calculated by solving simultaneously for $E_{\rm corr}$ using Eqs. (2-16), (2-17), and (2-20).

2.3.3.2 Critical Potentials for Pitting, Crevice Corrosion, and Stress Corrosion Cracking

Empirically derived equations are used in the present code for the dependence of critical potentials on environmental parameters. The pit initiation and repassivation potentials are assumed to depend only on the chloride concentration and temperature. Experimental results have shown that the dependence of critical potentials on pH, bicarbonate, and silica is negligible. As mentioned before, nitrate and sulfate can act as inhibitors if the ratio of nitrate to chloride or sulfate to chloride are sufficiently high (Sridhar et al., 1993). However, in the current calculations, the effects of these anionic species are not considered. The dependence of the critical potentials on chloride concentration and temperature is given by

$$E_{\rm crit} = A(T) + B(T) \log [C1^{-}]$$
 (2-22)

where the constants A(T) and B(T) were considered as linear functions of temperature. The constants were evaluated from literature and CNWRA data for initiation and repassivation potentials for both pitting and crevice corrosion (Sridhar et al., 1993).

Although the existence of a critical potential for stress corrosion cracking is less certain, it was assumed that is equal to the repassivation potential for localized corrosion. Justification for this assumption can be found in recent investigations (Tamaki et al., 1990; Tsujikawa et al., 1994), as discussed previously (Sridhar et al., 1993).

2.3.4 Mechanical Failure Models

The SCCEX code includes three mechanical failure models: buckling, yielding, and fracture. Simplified analytical models were developed to convert a seismic type load to a pseudostatic pressure acting on the curved shell surface of a container emplaced in an oversized vertical borehole. To generate the seismic load, it was assumed that the peak seismic acceleration would cause the container mass to impact the top part of the wall of the borehole, as shown in Figure 2-4a. Further, it was assumed that there were no momentum losses in the impact and the bottom of the container moved on a frictionless surface. The area of contact between the container and the borehole is shown in Figure 2-4b. In the calculations an arc length AB, the region of contact with the borehole, is assumed to be 10 percent of the circumference of the container. The load acts along a 10-cm length on the top part of the container. This is a conservative assumption considering that the entire impact load of the container is applied to a limited part of the container surface. Based on the peak acceleration, a uniform pressure, q, was calculated and used in the different mechanical models. In the deterministic analyses an acceleration of 0.4 g was used.

2.3.4.1 Buckling Failure Model

The model used in the analysis for buckling is described in Sridhar et al. (1993). In this model, a shell buckling case is considered where the arc AB is loaded with a pressure q as shown in Figure 2-5a. The analytical equation used for this model is reproduced as Eq. (2-23).



Figure 2-4. Schematic diagrams showing the contact between the container and the borehole: (a) side view; (b) top view





maximum stress applied at center of the beam



t = thickness of cylinder W = width of contact

(b)

Figure 2-5. Schematic diagrams showing the assumptions in the different mechanical models: (a) loading for buckling failure; (b) stresses for yield or fracture failure

r = radius of cylinder
alpha = central angle
q = uniform presure
AB = 1/10th of the circumference
C = center of cylinder



$$R_B = \frac{99Et_R^3 \pi}{60r^2(1 - v^2)}$$
(2-23)

where

- R_B = residual buckling load capacity for the container
- E = Young's Modulus
- \mathbf{v} = Poisson's ratio
- r = inner radius of the container
- t_R = remaining thickness at any given time after accounting for corrosion of the container

It should be noted that the constants in the expression are based on the initial thickness-to-radius ratio of the container being 1:10. A factor of safety equal to two was used for this failure model to add conservatism.

2.3.4.2 Yield Failure Model

The conceptual model for developing maximum stresses in the body of the container is shown in Figure 2-5b. Here it is assumed that the arc AB length of the container where the constant pressure q is applied, acts as a simply supported beam with a thickness equal to the wall of the container and a width of 10 cm. In the conceptual model, no credit is taken for any shell constraint in the axial direction of the container. However, the simply supported beam assumption may not be fully justified, particularly when some rigidity can be provided by the end caps of the container. The fixity at the end caps is not absolute and there is a degree of rotation and rigid body motion in the area. In future evaluations, detailed numerical stress analysis of the region is needed to scope the degree of conservatism in the current analysis. The moment developed on the simply supported beam was calculated and the appropriate maximum stress determined. The residual yield capacity, R_r , was determined (Sridhar et al., 1993) from the following equation.

$$R_{Y} = R_{YO} \frac{A_R}{A} = R_{YO} \frac{t_R}{t}$$
(2-24)

where

 R_{YO} = yield strength of the material A = initial cross section area of the solid part of the cylinder A_R = remaining cross section area of the solid part of the cylinder t = initial thickness of the cylinder t_R = remaining thickness of the cylinder after corrosion A factor of safety of two was also incorporated into Eq. (2-24) to permit conservative calculations.

2.3.4.3 Fracture Failure Model

The conceptual model for developing the stresses for fracture is the same as that described in the previous section. The fracture model is expressed (Sridhar et al., 1993) as

$$R_F = \frac{K_{\rm Ic}}{Y(\pi a)^{0.5}}$$
(2-25)

where

 R_F = permissible external stress Y = geometry factor a = crack depth or the depth of a corroded pit K_{1c} = fracture toughness

A factor of safety of two was used for this failure model to account for added conservatism.

2.3.4.4 Time-Dependent Thickness Models

An important parameter used in the buckling failure model and the stress computations is the time-dependent thickness of the container wall. It should be noted that the wall thickness is reduced as a result of general or local corrosion. In the case of general corrosion, the thickness is assumed to decrease uniformly with time. However, for localized corrosion effects the reduction of thickness is not uniform. To account for the nonuniform behavior of localized corrosion, a scheme was developed to approximate an average thickness reduction for the container. The approach is shown in Figure 2-6. It is assumed that pits or crevices develop in any wetted region on the surface of the container if the conditions discussed in Section 2.3.3.2 are fulfilled. Assuming the existence of a large number of pits or crevices in this region, the total volume of material reduced by corrosion is considered to be the volume of a right circular cone with the wetted area as the base and a height equal to the maximum pit depth calculated from the active corrosion rate at any given time. An average remaining thickness is calculated by distributing the volume reduction over the wetted surface.

2.4 EXAMPLE PROBLEM TEST CASES

Deterministic and probabilistic calculations were conducted for evaluating the performance of several container materials under different environmental conditions. These calculations were performed to predict lifetime of the containers by evaluating the time-to-failure as a result of the various postulated degradation modes. All the SCCEX code deterministic and probabilistic test runs for the different cases analyzed are summarized in Table 2-1. The baseline case is represented by an uncontrolled environment, resulting from the process of water evaporation and salt concentration from groundwater on the container surface described in Section 2.4.2, and the use of type 304L stainless steel (SS), which is considered the reference material in the SCP (U.S. Department of Energy, 1988b), as container material. Thermal







Assumed corroded volume = (1/3) x wetted area x Lmax

Lmax = CA = max. corroded depth

(b**)**

Figure 2-6. Schematic diagram showing the thickness reduction scheme for localized corrosion

Cases	Objective	Material	Environment	Deterministic Analysis	Probabilistic Analysis
Baseline	Reference material. Uncontrolled environment.	Type 304L SS	Uncontrolled Cl ⁻ concentration. High, intermediate, and low thermal power density.	10-yr fuel age. Parametric study of thermal power density. Parametric study of other input parameters (bounding cases).	10- to 60-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.
Alt-1	Alternative material. Uncontrolled environment.	Alloy 825	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	10-yr fuel age. Baseline case for input parameters.	10- to 60-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.
Alt-2	Reference material. Controlled environment.	Type 304L SS	Controlled Cl (<100 ppm) concentration. Intermediate thermal power density.	10-yr fuel age. Baseline case for input parameters.	10- to 60-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.
Alt-3	Alternative material. Controlled environment.	Alloy 825	Controlled Cl^- (<100 ppm) concentration. Intermediate thermal power density.	10-yr fuel age. Baseline case for input parameters.	10- to 60-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.

Table 2-1. Summary of example problem test cases

Table 2-1. Su	mmary of example	e problem test	cases	(cont'd)
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Cases	Objective	Material	Environment	Deterministic Analysis	Probabilistic Analysis
Alt-4	Highly designed material. Uncontrolled environment.	x	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	10-yr fuel age. Baseline case for input parameters.	10- to 60-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.
Alt-5	Highly designed material. Uncontrolled environment.	Y	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	10-yr fuel age. Baseline case for input parameters.	10- to 60-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.
Alt-6	Super designed material. Uncontrolled environment	Z	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	10-yr fuel age. Baseline case for input parameters.	30-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.
SS: CDF: PDF:	Stainless steel Cumulative distribution function Probability density function				

2-23

loading conditions represented by high, intermediate, and low thermal power density were considered in the definition of the evolution of the repository environment with time. In the deterministic analysis, a 10-yr-old spent fuel was used, whereas the age was varied from 10 to 60 yr for the probabilistic analysis. A more detailed explanation of the last two columns in Table 2-1 will be given when the results of the deterministic and probabilistic analyses are presented and discussed in Chapters 4 and 5, respectively.

An alternative case is represented by the use of alloy 825 as an alternative container material. This is one of the alloys selected by the DOE for additional investigations during the period of the advanced conceptual design of the waste package (van Konynenburg et al., 1993). Additional alternative cases are those in which a controlled environment was assumed to exist in contact with the container. This controlled environment was specifically defined by the arbitrary assumption that chloride, which is the predominant anion implicated in localized corrosion and stress corrosion cracking of Fe-Cr-Ni alloys (Cragnolino and Sridhar, 1991; 1992), cannot reach a concentration higher than 100 ppm $(2.8 \times 10^{-3} \text{ mol/kg water})$. This assumption reflects a condition where the refluxing water is essentially distilled water that dilutes the salt solution formed due to evaporation. It should be noted that the chloride concentration measured in J-13 well water, which is the reference water for the Yucca Mountain project, is equal to 6 ppm (Glassley, 1986).

In addition, three hypothetical materials, named X, Y, and Z, were considered in other alternative cases. These materials are characterized by distinctive mechanical properties and widely different resistance to specific degradation modes in the presence of the uncontrolled repository environment. Material X is a material with a relatively high uniform corrosion rate but extremely resistant to localized corrosion (pitting and crevice corrosion) and to stress corrosion cracking. Material Y is an alloy resistant to both general corrosion and localized corrosion, but susceptible to stress corrosion cracking within a specific potential range. Finally, material Z represents a material with good mechanical properties (high yield strength and high fracture toughness) and very good resistance to all forms of corrosion.

Additional alternative cases, representing secondary variations of the cases listed above, are summarized in Table 2-2. The initial variation is represented by a constant 30-yr fuel age instead of 10-yr for the deterministic analysis or the 10- to 60-yr range used for the probabilistic analysis. Another variation was the use of a modification of material Z, named Z^{I} , with an improved corrosion resistance.
Cases	Objective	Material	Environment	Deterministic Analysis	Probabilistic Analysis
Baseline-A	Reference material. Uncontrolled environment.	Type 304L SS	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	30-yr fuel age. Baseline case for input parameters	30-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.
Alt-3-A	Alternative material with improved corrosion resistance. Controlled environment.	Alloy 825	Controlled Cl ⁻ (<100 ppm) concentration. Intermediate thermal power density.	30-yr fuel age. Baseline case for input parameters. Parametric study of thermal power density.	30-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.
Alt-6-A	Super designed material. Uncontrolled environment.	Z	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	30-yr fuel age. Baseline case for input parameters.	30-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.
Alt-6-B	Super designed material with improved corrosion resistance. Uncontrolled environment.	Z ¹	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	30-yr fuel age. Baseline case for input parameters.	30-yr fuel age. 100 vectors. CDF and PDF for failure time vectors.

Table 2-2. Summary of additional alternative test cases for example problem

3 MODEL INPUTS

The parameters included in the SCCEX code input file for the different calculations and models were selected from applicable data available in the literature or estimated for particular processes (i.e., binary diffusion of water vapor through air, oxidation rate in air) on the basis of approximations to similar cases. Most of the parameters referring to the dimensions of the container and thermal properties for the near field environment were obtained from the SCP for the proposed repository at Yucca Mountain (U.S. Department of Energy, 1988a).

3.1 THERMAL AND ENVIRONMENT PARAMETERS

According to the SCP (U.S. Department of Energy, 1988b), the size of the container for the reference waste packages containing spent fuel is 4.76 m in height, with a radius of 0.33 m and a wall thickness of 0.01 m. In addition, the air gap was considered to be 0.01 m in the borehole in which the containers will be vertically emplaced according to the reference design. The outer boundary for the thermal calculations was assumed in this report to be located at 5.0 m. This is a somewhat arbitrary choice and future work will attempt to provide a more general treatment which removed this arbitrariness. For all the thermal calculations it was assumed that there are 70,000 metric tons of uranium (MTU) as pressurized water reactor (PWR) (60 percent) and boiling water reactor (BWR) (40 percent) spent fuel in the whole repository and 2.3 MTU per container. Data from the U.S. Department of Energy (1987) for the power output for each type of spent fuel as a function of time, expressed in W/MTU, were used in these calculations assuming the standard burnups of 33,000 and 27,500 MWd/MTU for PWR and BWR fuels, respectively. The input parameter is the age of the fuel that was varied uniformly from 10 to 60 yr in the initial probabilistic analysis but maintained constant at 30 yr in the last set of test cases (Table 2-2). The vertical dimension of the repository was assumed to be 4.0 m.

Among the thermal parameters, the initial power density was calculated from the repository thermal loading selected in the SCP (U.S. Department of Energy, 1988b). Using a value of 57 kW/acre, an initial power density of 4.44×10^8 J/m²/yr was calculated as an input for the baseline case considered to be the intermediate thermal loading in this report. A sensitivity analysis was conducted in which the initial power density was varied from 2.2×10^8 to 5.92×10^8 J/m²/yr (28.2 to 76.0 kW/acre) defining a range extended from low to high thermal loadings for the purpose of this report. The thermal conductivity of the rock was assumed to be 5.68×10^7 J/°K/m/yr (1.8 W/m/°K), which is similar to average values reported for saturated tuff samples (U.S. Department of Energy, 1988c). The thermal conductivity of the packing was considered to be about two-thirds of the rock thermal conductivity. In the case of the probabilistic analysis, ranges extended from 4.7×10^7 to 6.8×10^7 J/°K/m/yr and from 2.7×10^7 to 4.8×10⁷ J/°K/m/yr were used for the rock and the packing, respectively. For all the parameters, a uniform type of distribution within the selected range was used for the probabilistic analysis with few exceptions which will be specifically mentioned. An increase or decrease of approximately 20 percent around the value adopted for the base case was considered representative of the expected variations for this parameter in the case of the rock. A slightly higher variation (26 percent) was used for the thermal conductivity of the packing. It should be noted that, in the thermal analysis, the air gap in the SCP reference design was assumed to be partially filled with crushed tuff rock constituting for all purposes a packing. An effective thermal conductivity of 3.26×10^6 J/°K/m/yr was calculated for the container, using the approach suggested by Manteufel and Todreas (1992).

The volumetric heat capacity, calculated as the product of the density by the heat capacity, was assumed to have an average value of 2.4×10^6 J/m³/°K for all the rock, whereas it was considered for both the packing and the container to be half of that for the rock. The value adopted is reported in the SCP (U.S. Department of Energy, 1988c) as a calculated value for a saturated rock with a porosity of 0.10 and a grain density of 2.65 g/cm³. The range of variation selected in the probabilistic analysis (2.2×10^6 to 2.6×10^6 J/m³/°K) reflects a variation in porosity from 0.0 to 0.2, according to the estimations presented in the SCP (U.S. Department of Energy, 1988c).

For the parameters related to the evaporation process, a binary diffusion coefficient of water vapor in air was assumed, according to the expression given by Treybal (1980), to calculate the coefficient at the temperature of interest

$$D(m^2/s) = 3.05 \times 10^{-5} (1/p) (T/T_{ref})^{3/2}$$
 (3-1)

where p, the pressure at the repository horizon, is equal to 0.895 bar in comparison to the normal value of 1 bar and the reference temperature T_{ref} is expressed in °K. A value of 962 m²/yr was calculated as input parameter at the reference temperature of 232 °K (59 °C).

A porosity of the rock and the packing equal to 0.12 was adopted, with a range for the probabilistic analysis extended from 0.05 to 0.2, only in the case of the rock. While a tortuosity factor for the rock and the packing equal to 1.0 was used in the baseline case, a range from a low value of 0.01 to 1.0 with a log uniform distribution was adopted for the probabilistic studies in the case of the rock, on the basis of the discussion presented by Jury et al. (1991). The thickness of the liquid water film formed on the surface of the container was assumed to vary from 1 to 3 mm in the probabilistic analysis, whereas 2 mm, which seems to be a reasonable value, was chosen for the baseline case in the deterministic analysis. A water drip rate of 1×10^{-3} m³/yr was arbitrarily selected as input parameter, with a water salt concentration of 0.0613 kg/m³ on the basis of the concentration of Cl⁻, NO₃⁻, Na⁺, and K⁺ reported for J-13 well water (U.S. Department of Energy, 1989). A scale content in the dripping water of 0.2121 kg/m³ was used, by considering that HCO_3^- , SO_4^{2-} , SiO_2 , Ca^{2+} , and Mg^{2+} present in J-13 well water are scale formers. For the probabilistic analyses of the overall system, however, ranges of 0.05 to 0.2 kg/m³ and 0.0 to 0.5 kg/m³ were selected for the salt concentration and the scale concentration, respectively, assuming that the interaction of water with minerals coupled to several solution concentration processes can modify the composition of the dripping water. It should be noted that in the example analysis, only the "umbrella" option was exercised. The flow rate may be an important parameter if other options are included. This will need further model development in the future. To account for the formation of concentrated solutions of salts other than NaCl, the scale factor for vapor pressure lowering relative to a saturated NaCl solution concentration factor was varied from 0.7 to 1.3, whereas a value of 1.0, corresponding to NaCl as a single salt, was chosen in the deterministic analysis for the baseline case. However, regardless of the scale factor, only NaCl was considered for the corrosion models. A solubility of NaCl equal to 27.5 weight percent at 100 °C was adopted (Linke, 1965). The initial amount of salt was varied in the probabilistic analysis from 0.0 to 5.0 kg and that of the scale from 0.0 to 15.0 kg. The initial amount of salt was selected to be 0.1 kg in the deterministic analysis for the baseline case, but no initial scale was assumed in this case.

Although a value of the water drip rate was selected as input parameters, most of the calculations were performed using the umbrella option. This is the case in Table B-1 (Appendix B), where

the SCCEX Input File for the baseline case is shown. Additional parameters related to the back flow of liquid water towards the container are those characterizing the hydrothermal umbrella formed on top of the repository. This group of parameters includes the umbrella edge thickness, the umbrella edge temperature, and the range of temperatures around the umbrella edge temperature. These parameters were varied in the probabilistic analysis from 1.0 to 30.0 m, 90.0 to 98.0 °C, and 0.1 to 5.0 °C, respectively, whereas values of 20 m, 95 °C, and 2 °C were used in the deterministic analysis for the baseline case. An additional parameter is the funnel area which was varied from 0.1 to 10.0 m² with a log uniform distribution for the probabilistic analysis. A value of 1.0 m² was selected as the baseline case for the deterministic analysis. The values assigned to these parameters are based in reasonable assumptions within the context of the postulated model. Obviously, they cannot be independently verified.

All the values of the parameters used in the input file of the SCCEX code for the deterministic analysis (baseline case) and the ranges and type of distribution for the probabilistic analyses are summarized in Table 3-1.

3.2 CORROSION POTENTIAL PARAMETERS

Another group of parameters is that related to the corrosion processes which can be classified in two subgroups. The first subgroup includes all the parameters needed for the calculation of the corrosion potential.

For the cathodic reaction corresponding to oxygen reduction, the mass transport parameters of importance are the diffusion coefficient and the solubility of oxygen in solution. The oxygen solubility is expressed in terms of the Henry's law constant, which is given as a function of temperature by

$$ln K_{H} = 0.2984 - 5.59617 \times 10^{3}/T + 1.04967 \times 10^{6}/T^{2}$$
(3-2)

where K_H is the Henry's constant in moles/kg/atm and T is the temperature in °K, according to Battino (1981). The diffusion coefficient of oxygen at any temperature was calculated from

$$D = 0.063 \exp \{ (14.644/R) [(1/298.15) - (1/T)] \}$$
(3-3)

where D is the diffusion coefficient in m²/yr, and R is the ideal gas constant expressed in kJ/mol/°K. The pre-exponential coefficient and the activation energy were calculated from the experimental data reported by Case (1973).

Additional parameters that are relevant to this calculation are those related to the diffusion path for oxygen. Since in the model both the porosity and the tortuosity of the scale may affect the value of the corrosion potential if mass transport of oxygen is rate controlling, these parameters were varied from 0.1 to 1.0 and 0.2 to 1.0, respectively. These two parameters can be lumped together since the product of both by the diffusion coefficient defines an effective diffusion coefficient for the diffusion of oxygen through the pores of the scale towards the metal surface. Values of 0.3 for tortuosity and 0.5 for porosity were adopted in the deterministic analyses for the baseline case, resulting in an effective diffusion coefficient that is 15 percent of the diffusion coefficient in the bulk solution.

	Deterministic Analysis	Probabilistic Analysis		
Parameters	Baseline Case	Range	Type of Distribution	
Age of fuel, t (yr)	10	10.0 to 60.00	Uniform	
Thermal conductivity of rock, <i>tkr</i> (J/yr/m/°K)	5.7×10 ⁷	4.7×10^7 to 6.8×10^7	Uniform	
Thermal conductivity of packing, <i>tkp</i> (J/yr/m/°K)	3.8×10 ⁷	2.7×10^7 to 4.8×10^7	Uniform	
Volumetric heat capacity of rock, <i>rhocpr</i> (J/m ³ /°K)	2.4×10 ⁶	2.0×10^6 to 3.0×10^6	Uniform	
Tortuosity of rock, taur	1.0	0.01 to 1.0	Log uniform	
Porosity of rock, phir	0.12	0.05 to 0.2	Uniform	
Water film thickness, delta (m)	2.0×10 ⁻³	1.0×10^{-3} to 3.0×10^{-3}	Uniform	
Salt concentration, salt (kg/m ³)	0.0613	0.05 to 0.2	Uniform	
Scale concentration, scale (kg/m ³)	0.2121	0.0 to 0.5	Uniform	

Table 3-1. Values of input parameters for thermal and environmental models

	Deterministic Analysis	Probabilistic	Analysis
Parameters	Baseline Case	Range	Type of Distribution
Vapor pressure lowering scale factor, bfact	1.0	0.7 to 1.3	Uniform
Initial salt, <i>dsalt</i> (kg)	0.1	0.0 to 5.0	Uniform
Initial scale, <i>dscale</i> (kg)	0.0	0.0 to 15.0	Uniform
Funnel area, <i>dfrac</i> (m ²)	1.0	0.1 to 10.0	Log uniform
Umbrella edge thickness, <i>slice</i> (m)	20.0	1.0 to 30.0	Uniform
Umbrella edge temperature, <i>tenhan</i> (°C)	95	90.0 to 98.0	Uniform
Range of umbrella edge temperature, <i>tslop</i> (°C)	2.0	0.1 to 5.0	Uniform

Table 3-1. Values of input parameters for thermal and environmental models (cont'd)

ა ა The parameters of the Butler-Volmer equation for the current density as a function of potential corresponding to the oxygen reduction reaction are the transfer coefficient (β), the rate constant (k_{O_2}), and the activation energy. Values ranging from 0.25 to 1.5 with a uniform distribution were assigned to β for the initial probabilistic analysis, but in the baseline case, and in most of the subsequent test cases, a constant value of 0.75 was used. This value is half of the one suggested by Macdonald and Urquidi-Macdonald (1990). These authors indicate that, among other adjustments, the transfer coefficient for the oxygen reduction reaction was modified from 0.5 to 1.5 in order to obtain reasonable values of the redox potential, fulfilling the condition $-1.0 < E_{redox} < 1.0 V_{SHE}$ (Urquidi-Macdonald et al., 1990). The value of β is slightly higher than that of 0.5 reported by Vetter (1967), but lower than $\beta = 1.0$ as reported by Damjanovic (1969), in both cases for the reduction of oxygen on oxide-free platinum. Recent data of Okuyama and Haruyama (1990) for SS in a borate buffer solution exhibited a Tafel slope of 60 mV/decade for the reduction of oxygen which implies a transfer coefficient of 1.0. The use of $\beta = 0.75$ seems to be a reasonable compromise until more accurate data can be obtained.

The rate constant was varied from 3.0×10^6 to 3.0×10^{14} C·m/(mol·yr) in the initial probabilistic analysis, in which a uniform distribution was used. However, further test cases were conducted using a range reduced from 3.0×10^8 to 3.0×10^{12} C·m/(mol·yr) that seems more realistic for a passive metal of the iron-group (Bockris and Reddy, 1970). A constant value of 100 kJ/mol was adopted for the activation energy according to Macdonald and Urquidi-Macdonald (1990).

It should be noted, however, that the value selected for β has a very strong effect on the value of the exchange current density, $i_{O_2}^0$, the parameter usually reported in the literature instead of the rate constant, k_{O_2} . With the values of β and k_{O_2} used in the computations, very low values of $i_{O_2}^0$ are obtained. If values of $i_{O_2}^0$ more close to those reported for noble metals in acidic media (10⁻¹⁰ to 10⁻¹² A/cm²) are used, the corrosion potential would acquire highly positive values (>0.6 V_{SHE}) which cannot be considered realistic in an aerated environment in the absence of more powerful oxidants than molecular oxygen.

For the cathodic reduction of water, β was varied from 0.25 to 0.5 in the initial set of probabilistic analyses (uniform distribution), but for later test cases a constant value of 0.5 was maintained, as commonly reported (Vetter, 1967; Bockris and Reddy, 1970) for the case of electrochemical discharge as rate determining step followed by chemical desorption. The rate constant was varied initially from 3.2×10^{-4} to 3.2×10^4 C/(yr \cdot m²), but the range was reduced from 3.2×10^{-2} to 3.2×10^2 C/(yr \cdot m²) in later test cases. The activation energy, however, was maintained constant assuming a value of 20 kJ/mol, according to the considerations of Macdonald and Urquidi-Macdonald (1990).

All the values of the parameters used in the input file of the SCCEX code are summarized in Table 3-2 for both the deterministic analysis (baseline case) and for the probabilistic analysis. For the probabilistic cases the ranges and type of distribution originally used are distinguished from the modified values adopted in later runs.

	Deterministic Analysis	Probabilistic Analysis					
		Ra	nge	Type of Distribution			
Parameters	Baseline Case	Initial	Modified	Initial	Modified		
Oxygen beta kinetics parameter, betaox	0.75	0.25 to 1.5	0.75	Uniform	Constant		
Water beta kinetics parameter, betahy	0.5	0.25 to 0.5	0.5	Uniform	Constant		
Rate constant for oxygen reduction, <i>rkox</i> [C • m/(mole • yr)]	3.0×10 ¹⁰	3.0×10^{6} to 3.0×10^{14}	3.0×10^8 to 3.0×10^{12}	Uniform	Uniform		
Rate constant for water reduction, <i>rkhy</i> [C/(m ² • yr)]	3.2	3.2×10^{-4} to 3.2×10^{4}	3.2×10^{-2} to 3.2×10^{2}	Uniform	Uniform		
Current density for air/steam, curair [C/(yr • m ²)]	6.3×10 ²	6.3 to 6.3×10^3	6.3 to 6.3×10^3	Uniform	Uniform		
Active current density, curact [C/(yr • m ²)]	6.3×10 ⁶	6.3×10^5 to 6.3×10^8	6.3×10^5 to 6.3×10^7	Uniform	Uniform		
Passive current density Cpass coefficient aa(1) [C/(yr • m ²)]	6.3×10 ⁴	6.3×10^3 to 6.3×10^5	6.3×10^3 to $6.3 \times 10^{5*}$	Uniform	Uniform		
Tortuosity factor for scale, taus	0.3	0.1 to 1.0	0.1 to 1.0	Uniform	Uniform		
Scale porosity, spor	0.5	0.2 to 1.0	0.2 to 1.0	Uniform	Uniform		
* Alt-3-A and Alt-6-B: 6.3×10^3 to 6.3×10^4							

 Table 3-2.
 Values of input parameters for corrosion models

3.3 GENERAL CORROSION, LOCALIZED CORROSION, AND STRESS CORROSION CRACKING PARAMETERS

During the time prior to the wetting of the container surface, it was assumed that type 304L SS, which is the reference material for the example problem, is corroding in air with a very slow corrosion rate corresponding to the formation of a thin oxide film. It was assumed that the metal/oxide interface recedes at a rate equivalent to 6.3×10^2 C/(yr \cdot m²), which is about 0.02 μ m/yr. The range adopted in the probabilistic analysis extended from 6.3 to 6.3×10^3 C/(yr \cdot m²). Corrosion or oxidation rates ranging from 0.07 to 0.2 μ m/yr were reported by McCright et al. (1987) for type 304L SS in contact with groundwater or water vapor at about 100 °C, even in the presence of γ -radiation. These values are in close agreement with older data reported in the literature.

For the consideration of the anodic corrosion process that occurs as soon as the container surface is wetted, a rate of dissolution in the presence of an aqueous solution equivalent to a passive current density of the order of 2×10^{-7} A/cm² (approximately 2 μ m/yr) can be assumed for a corrosion-resistant alloy such as type 304L SS (Sedriks, 1979). A range varying from 6.3×10^3 to 6.3×10^5 C/(yr · m²) was used in the probabilistic analysis and 6.3×10^4 C/(yr · m²), which is equivalent to 2 μ m/yr, for the baseline case in the deterministic analysis. In a test case in which a corrosion allowance material designated as X was analyzed as an alternate material, the current density was increased to values ranging from 1.2×10^6 to 1.3×10^6 C/(yr · m²) to reflect a reasonably higher rate of general corrosion of the order of 40 μ m/yr.

For the consideration of localized corrosion, the dependence of the critical potentials for initiation (E_p) and repassivation (E_{rp}) on chloride concentration and temperature were previously discussed in detail (Sridhar et al., 1993). A general expression for both parameters of the form

$$E_{\rm crit} = A(T) + B(T) \log [C1^{-}]$$
 (3-4)

was established on the basis of extensive literature data, in which the constants A(T) and B(T) were found to be linear functions of the temperature expressed in °C (Sridhar et al., 1993).

For type 304L SS, which is the reference material for the analysis, the following relationships were used for E_p

$$A(T) = 187.4 - 3.7 T (^{\circ}C) ; B(T) = -76 + 0.06 T (^{\circ}C)$$
 (3-5)

and for E_{rp}

$$A(T) = -172.4 - 2.4 T (^{\circ}C); B(T) = -80.1 + 0.35 T (^{\circ}C)$$
 (3-6)

For alloy 825, considered as alternate material in some test cases, the following parameters were used for E_p

$$A(T) = 200 \text{ for } T \ge 50^{\circ}\text{C} ; B(T) = -120 \text{ for } T \ge 50^{\circ}\text{C}$$
 (3-7)

and for E_{rp}

$$A(T) = 346.5 - 6.7 T(^{\circ}C); B(T) = 76.3 - 1.9 T(^{\circ}C)$$
 (3-8)

In all these equations, A(T) and B(T) are expressed in mV_{SCE} (saturated calomel electrode scale) and mV/decade, respectively. The resulting values of E_p and E_{rp} are converted to V_{SHE} (standard hydrogen electrode scale) for comparison with E_{corr} values.

For another alternate material, denoted Z, which was considered in some test cases as an alloy with extremely high resistance to localized corrosion in highly concentrated chloride-containing solutions (e.g., C-22/C-276/C-4), a very high initiation potential, $E_{\rm crit} = 0.8 V_{\rm SHE}$, was adopted as an input parameter in the code even at very high chloride concentrations.

When the corrosion potential becomes higher than the critical potential for initiation of localized corrosion, it is assumed that localized corrosion in the form of pitting occurs instantaneously without an induction time and the localized corrosion rate acquires values typical of slow active dissolution. For the deterministic analysis, a value of 6.3×10^6 C/yr \cdot m² (2×10^{-5} A/cm²) was used for the baseline case, whereas a range of 6.3×10^5 to 6.3×10^8 C/yr \cdot m² was used in the probabilistic analysis. Values ranging from 6.3×10^5 to 6.3×10^7 were adopted in the last set of test cases.

The approach adopted for the consideration of stress corrosion cracking failures is based on two assumptions. The first is that the stress intensity, K_I , at an existing flaw on the container has to exceed K_{Iscc} , which is a material- and environment-dependent parameter. The second assumption is that the controlling factor for the occurrence of stress corrosion cracking is the potential, which must be higher than E_{rp} . For type 304L SS and alloy 825, K_{Iscc} is relatively high. Therefore, stress corrosion cracking will not compete with localized corrosion for the test cases in which these alloys were considered. To determine the effect of stress corrosion cracking, a material with a very high yield strength, named Y, which exhibits a very low K_{Iscc} and a relatively low K_{Ic} , was considered an alternative material. The controlling factor for the occurrence of stress corrosion cracking in this material was the potential. It was assumed that cracking occurs within the range of potentials defined by E_{rp} and E_p after an initiation or induction time of 20 yr. Subcritical crack growth was postulated to occur with a crack propagation rate of 5.0×10^{-4} m/yr, independent of stress intensity, which is characteristic of Stage II cracking. No dependence of the crack growth rate on potential was considered, but this is a relatively well established feature in many alloy/environment systems at relatively high potentials with respect to the critical potential for stress corrosion cracking (Cragnolino, 1985).

The range of potentials selected in this example was defined by the following expressions.

$$E_p (\mathrm{m}V_{\mathrm{SCE}}) = 400 - 90 \log [Cl^{-}]$$
 (3-9)

$$E_{rp} (mV_{SCE}) = (600 - 7.0T) + (80 - 2.0T) \log [Cl^{-}]$$
 (3-10)

where T is temperature in °C, with the bounding condition that $E_{p} < \Delta E_{scc} < E_{p}$, where ΔE_{scc} is the potential range for stress corrosion cracking of material Y in high-temperature chloride-containing solutions.

3.4 MECHANICAL PARAMETERS

The mechanical properties of the alloys, considered in this study as input for the mechanical failure models, are listed in Table 3-3. It was assumed that type 304L SS, alloy 825, material X, and material Z have the same mechanical properties but different corrosion characteristics, as discussed in Section 3.3. On the other hand, for material Y, a relatively low fracture toughness but a very high yield strength was assumed.

Material	304L SS	Alloy 825	X	Y	Z
Yield Strength (MPa)	170	170	170	1,650	170
Young's Modulus (MPa)	1.82×10^{5}	1.82×10^{5}	1.82×10^{5}	2.1×10 ⁵	1.82×10^{5}
Poisson's ratio	0.25	0.25	0.25	0.25	0.25
Fracture toughness (MPa • m ^{1/2})	300	300	300	40	300

Table 3-3. Mechanical properties of materials included in this study

All material properties were assumed to be constant in both deterministic and probabilistic analyses. However, these properties, with the exception of the fracture toughness, were considered to be temperature dependent. The mechanical properties at the temperature of interest were considered to be equal to those at room temperature (20 °C) multiplied by temperature-dependent functions. These functions (IPA, 1993) are listed in Table 3-4 for type 304L SS. No temperature correction was applied to fracture toughness. For the other materials, the same temperature-dependent functions were applied.

Properties at Temperature $T =$ (Properties at 20 °C)× $f(T)$	Temperature Function, f(T) T: °C
Yield Strength (MPa)	$1 - 10^{-3} (T - 20)$
Young's Modulus (MPa)	$1 - 6 \times 10^{-4} (T - 20)$
Poisson's ratio	$1 + 4 \times 10^{-4} (T - 20)$

 Table 3-4. Temperature corrections for mechanical properties

4 DETERMINISTIC ANALYSES

As noted in Chapter 2, Tables 2-1 and 2-2 summarize all the test runs performed with the SCCEX code. As part of the deterministic analyses, a parametric study of the effect of thermal power density was conducted for the baseline case, followed by a study of the effect of varying the values of the input parameters (bounding cases). Many alternative cases in terms of the container material and the characteristics of the environment (uncontrolled or controlled) were also considered. All these test runs are discussed in the following.

4.1 PARAMETRIC STUDY OF THERMAL POWER DENSITY

The influence of thermal loading on the performance of the waste package is undoubtedly very important. The conceptual approach of the DOE to the design of the repository at Yucca Mountain rests on the hypothesis that by selecting an appropriate thermal loading strategy it is possible to maintain a dry environment in the surroundings of the containers, consisting only of hot air, during a time interval that can be extended well beyond the regulatory containment period.

Several runs were conducted, as summarized in Table 4-1, to evaluate the effect of the initial power density on the time at which the container is wetted (termed time-to-wetting or wetting time). For the baseline case, in which type 304L SS is the container material in an uncontrolled environment and the value of the input parameters are those defined for the base case in Chapter 3 (Table 2-1), it can be seen that a minimum in the wetting time of about 725 yr occurs at initial thermal power densities ranging from 4.7×10^8 to 5.0×10^8 J/m²/yr. This range is slightly above the value of 4.44×10^8 J/m²/yr, or 57 kW/acre, which is designated as intermediate thermal loading in this report, and corresponds to the value adopted by the DOE in the SCP. The effect of high thermal loading is clearly seen in Figure 4-1, where it is noted that the wetting time rapidly increases above 5.0×10^8 J/m²/yr until it exceeds 1,000 yr, which is the maximum time selected for these simulations. The increased wetting period above 5.0×10^8 J/m²/yr represents a more extended period above the boiling point of the solution on the container surface. At lower power density, the trend is more complex and the minimum described above results from the interaction of two competing processes.

As discussed in Chapter 2, evaporation/condensation from/to the container results from the differences in vapor pressure between the solution on the container surface and the water present in rock pores or fractures at a certain distance from the container surface. In the model, two competing phenomenon are assumed to control the vapor pressure. The temperature gradient near the container causes an elevation of the vapor pressure of water on the container surface. On the other hand, soluble salt buildup on the container surface causes a lowering of vapor pressure. Both phenomena are temperature-dependent. The vapor pressure change arising from temperature depends on the average temperature gradient around the waste package. The temperature gradient around the waste package declines with time as the radioactive waste decays, whereas the average temperature depends upon the initial areal loading and age of fuel. The temperature gradient around the waste package is not a function of the initial power density, only of the age of the fuel and the mass of fuel per container. However, the temperature gradient is also a function of the distance chosen as outer boundary, and this has an effect on the wetting time, as discussed in Section 4.2.

The effect of salinity on vapor pressure is also temperature-dependent and is greater at higher temperature. Walton (1993) calculated the ability of several saturated salt solutions to lower the vapor

Initial Thermal Power Density (J/m ² /yr)	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	t _f (yr)	Temp. at t _w (°C)
2.2×10 ⁸	>1,000	_		>1,000	60.0
2.4×10 ⁸	995	0.15	-0.12	>1,000	62.8
2.6×10 ⁸	965	0.15	-0.13	>1,000	66.1
2.8×10 ⁸	925	0.16	-0.13	965	69.4
2.96×10 ⁸	925	0.16	-0.13	975	71.7
3.2×10 ⁸	875	0.17	-0.15	915	75.8
3.5×10 ⁸	845	0.17	-0.16	885	80.6
3.8×10 ⁸	815	0.18	-0.17	855	85.4
4.1×10 ⁸	765	0.18	-0.18	815	90.7
4.44×10 ⁸	735	0.19	-0.19	795	96.3
4.56×10 ⁸	735	0.19	-0.20	795	98.1
4.7×10 ⁸	725	(-0.5, 0.18)	-0.20	785	100
4.85×10 ⁸	725	(-0.5, 0.18)	-0.20	865	103
5.0×10 ⁸	725	(-0.5, 0.18)	-0.20	>1,000	105
5.1×10 ⁸	805	(-0.5, 0.18)	-0.20	>1,000	105
5.2×10 ⁸	885	(-0.5, -0.28)	-0.20	>1,000	105

Table 4-1. Results for different initial thermal power densities for baseline case (304L SS containers under uncontrolled environmental conditions)

Initial Thermal Power Density (J/m ² /yr)	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	t _f (yr)	Temp. at t _w (°C)
5.3×10 ⁸	975	-0.50	-0.20	>1,000	105
5.6×10 ⁸	> 1,000	—	_	>1,000	109
5.92×10 ⁸	> 1,000			>1,000	113

Table 4-1. Results for different initial thermal power densities for baseline case (304L SS containers under uncontrolled environmental conditions) (cont'd)



Figure 4-1. Effect of the initial power density on the time-to-wetting and the time-to-failure for baseline case (type 304L SS in uncontrolled environment)

pressure of water sufficiently to overcome a temperature-induced pressure gradient and expressed the results in terms of an equivalent temperature drop attributable to the salt solution. These results indicate that the solute effects increase with temperature. At lower thermal power loading, the temperature gradient depends only on time, whereas the salinity effect increases with temperature. This causes a decrease in the wetting time at higher average temperatures associated with moderate thermal loading. This trend continues until extended periods above the boiling point are encountered above $5 \times 10^8 \text{ J/m}^2/\text{yr}$. Because of the simplified thermal model and the simplifying assumption about the vapor pressure of water at a certain distance from the container, it is difficult to ascertain that the predicted trend shown in Figure 4-1 would actually occur in a more complex repository situation. Also, as noted before, the wetting time values depend on the outer distance selected as input parameter and, therefore, changes in t_w can be expected if a more realistic thermal model is used.

The corrosion potential, E_{corr} , attained on the wetted metal surface at the wetting time, is listed in Table 4-1, together with the critical potential for the propagation of localized corrosion, E_{crit} . It should be noted that a conservative criterion was adopted in the deterministic calculations by using E_{rp} as E_{crit} . This means that even though a higher potential is required for initiation of localized corrosion, the bounding parameter for repassivation of localized corrosion which is also the minimum potential to maintain a pit propagating was selected as controlling parameter. As discussed before, localized corrosion was assumed to be initiated instantaneously (no induction time) when $E_{corr} > E_{crit}$. Failure of the container takes place when through-wall penetration of the container occurs over a very small area at a penetration rate similar to that corresponding to active corrosion. Therefore, the time at which throughwall penetration occurs is termed time-to-failure or failure time. As seen in Figure 4-1, a minimum failure time of 785 yr was observed at an initial thermal power density of 4.7×10^8 J/m²/yr. Wall penetration occurred in a 60-yr period after the container surface becomes wetted. It is noticeable in Figure 4-1, as well as in Table 4-1, that at high thermal power densities $(>4.85 \times 10^8 \text{ J/m}^2/\text{yr})$ the time required after wetting for penetration of the container wall, as a result of localized corrosion, increased to more than 275 yr. This increase in the lifetime of the container, although wetted, results from the variation of the corrosion potential between -0.5 and $0.18 V_{\rm SHE}$, which implies that $E_{\rm corr}$ was lower than E_{crit} over a significant time interval, extending, therefore, the life of the container over that observed at lower thermal power. The value of the temperature on the container surface at the time at which wetting occurs is also shown in Table 4-2. This temperature increases monotonically with increasing thermal power density.

For comparison purposes, the effect of initial power density was studied for 30-yr-old fuel, using alloy 825 as a container material with the assumption of a controlled environment in which the chloride anion concentration was maintained lower than 300 ppm $(8.5 \times 10^{-3} \text{ m})$. This can be accomplished, for example, by using an appropriate backfill with ion exchange properties for Cl⁻ anions. The results of the different runs are summarized in Table 4-2. Regardless of the container material and the control of the chemical composition of the environment, the main effect of fuel age is reflected in the wetting time. Wetting occurs at shorter times than in the previous case (705 yr in comparison to 725 yr), but over a narrower range of initial thermal power density and displaced towards the lower values of the range studied. This is clearly seen by comparing Figure 4-2 with Figure 4-1. At thermal power density higher than $3.9 \times 10^8 \text{ J/m}^2/\text{yr}$, the wetting time increases beyond the 1,000-yr period adopted as a limit for these simulations. As noted above, the simplifying assumptions in the thermal environmental model lead to time-to-wetting values which may change significantly by using a more realistic thermal model.

Initial Thermal Power Density (J/m ² /yr)	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	t _f (yr)	Temp. at t _w (°C)
1.5×10 ⁸	995	0.15	0.29	>1,000	58.9
1.8×10 ⁸	935	0.15	0.27	>1,000	65.0
2.15×10 ⁸	875	0.17	0.26	>1,000	72.1
2.5×10 ⁸	825	0.17	0.24	>1,000	79.2
2.8×10 ⁸	785	0.18	0.23	>1,000	85.3
2.96×10 ⁸	745	0.18	0.22	>1,000	88.5
3.1×10 ⁸	715	0.19	0.21	>1,000	93.3
3.3×10 ⁸	705	(0.18, -0.51)	0.21	>1,000	95.3
3.45×10 ⁸	705	(0.18, -0.53)	0.21	>1,000	96.7
3.525×10 ⁸	705	(0.18, -0.53)	0.21	>1,000	99.8
3.6×10 ⁸	765	(0.18, -0.53)	0.21	>1,000	101
3.7×10 ⁸	895	-0.53	0.20	>1,000	103
3.73×10 ⁸	945	-0.53	0.20	>1,000	104
3.77×10 ⁸	995	-0.53	0.20	>1,000	105
3.9×10 ⁸	>1,000			>1,000	107
4.44×10 ⁸	>1,000		<u> </u>	>1,000	118
5.92×10 ⁸	>1,000			>1,000	146

Table 4-2. Results for different initial thermal power densities for Alt-3-A case (alloy 825 containers under controlled environmental conditions)



Figure 4-2. Effect of the initial power density on the time-to-wetting for Alt-3-A case (alloy 825 in controlled environment)

It is also important to note in Table 4-2 that, although the corrosion potential of the container material, alloy 825 in this case, is relatively close, as expected, to that shown in Table 4-1 for type 304L SS, E_{corr} was always lower than E_{crit} for the propagation of localized corrosion on alloy 825. Therefore, localized corrosion did not occur despite the fact that the surface container was wet. The combination of a material with a better resistance to localized corrosion, as reflected in higher values for the parameters E_p and E_{rp} at any given chloride concentration, and the selection of a controlled chloride environment lead to the predicted absence of localized corrosion within the 1,000-yr period chosen for these simulations. The time interval after wetting without the occurrence of failure was increased over 295 yr as a result of the better corrosion resistance. However, by comparing the E_{corr} and E_{crit} values in Table 4-2 at each initial thermal power density, it can be concluded that with the exception of the region of high initial thermal power density $(>3.6\times10^8 \text{ J/m}^2/\text{yr})$, the difference between the critical potential for localized corrosion and the corrosion potential decreased from 140 mV to less than 30 mV with increasing thermal power density. Obviously, if such difference is reduced, for example by an increase in the chloride concentration causing a decrease in the value of E_{crit} , failure may become possible at more extended time periods. On the contrary, if radiolysis reactions leading to the formation of H_2O_2 are assumed, the resulting increase in E_{corr} may lead to premature failure of the container after wetting.

4.2 PARAMETRIC STUDY OF OTHER INPUT PARAMETERS

4.2.1 Thermal and Environmental Parameters

As indicated in Table 2-1, a study of the input parameters included in the SCCEX code was performed adopting the relevant variables of the baseline case. The input parameters studied are those listed in Table 2-1, in which the value adopted for the base case is included for comparison. The container material is type 304L SS, and no provisions were established to control the environment. The chloride concentration was calculated from the salinity of the solution involved in the vapor pressure lowering at the container surface. The consideration of salts other than NaCl is discussed below.

In Table 4-3, the results obtained are listed in which the relevant results of the code runs are expressed in wetting time (t_w in yr), corrosion potential (E_{corr} in V_{SHE}), critical potential (E_{crit} in V_{SHE}) and failure time (t_w in yr). It should be emphasized, however, that the values of the wetting time included in this table are very sensitive to the choice of the outer boundary in the thermal model for the calculation of the temperature drop between the container and the rock away from the container. By varying this distance, r_3 , from 2 to 9 m, the wetting time increases from 415 yr to 965 yr. For the value adopted in all the calculations, which is 5 m, the wetting time is 735 yr. This variation in wetting time is related to the variation in the temperature of the container surface at the time-to-wetting, since this temperature decreases from 99.4 °C to 93.8 °C when r_3 is varied from 2 to 9 m. In Table 4-3, the base case is represented by an astrick (*), and parameters varied one at a time.

4.2.1.1 Age of Fuel

The first input parameter analyzed was the age of the fuel at the time of emplacement. This parameter was varied from 10 to 60 yr. It is apparent from Table 4-3 that the wetting time increased with fuel age and fuel with an age equal or greater than 20 yr did not promote wetting of the container in a

Parameters	Parameter Values	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	<i>t_f</i> (yr)
Age of fuel, t (yr)	10* 15 18 20 30 60	735 745 965 > 1,000 > 1,000 > 1,000	0.19 -0.53† -0.53† 	-0.19 -0.20 -0.20 	795 > 1,000 > 1,000 > 1,000 > 1,000 > 1,000
Thermal conductivity of rock, <i>tkr</i> (J/yr/m/°K)	$\begin{array}{r} 4.7 \times 10^{7} \\ 5.7 \times 10^{7*} \\ 6.8 \times 10^{7} \\ 7.5 \times 10^{7} \end{array}$	925 735 605 545	0.19 0.19 0.19 0.18	-0.20 -0.19 -0.18 -0.18	985 795 645 595
Thermal conductivity of packing, <i>tkp</i> (J/yr/m/°K)	$2.7 \times 10^{7} \\ 3.8 \times 10^{7*} \\ 4.8 \times 10^{7}$	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	805 795 785
Volumetric heat capacity for rock, <i>rhocpr</i> (J/m ³ /°K)	$2.0 \times 10^{6} \\ 2.4 \times 10^{6*} \\ 2.8 \times 10^{6} \\ 3.0 \times 10^{6}$	725 735 765 805	0.18‡ 0.19 0.18 0.18	-0.21 -0.19 -0.18 -0.17	875 795 805 855
Tortuosity of rock, taur	0.01 1.0*	735 735	0.19 0.19	-0.19 -0.19	775 795
Porosity of rock, phir	0.05 0.12* 0.2	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	785 795 795

Table 4-3. Deterministic parametric study for thermal and environmental models

Parameters	Parameter Values	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	<i>t_f</i> (yr)
Water film thickness, <i>delta</i> (m)	$ \begin{array}{c c} 1.0 \times 10^{-4} \\ 1.0 \times 10^{-3} \\ 2.0 \times 10^{-3*} \\ 4.0 \times 10^{-3} \end{array} $	735 735 735 735 735	0.19 0.19 0.19 0.19	-0.19 -0.19 -0.19 -0.19	805 805 795 785
Salt concentration, salt (kg/m ³)	0.05 0.0613* 0.2	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	795 795 785
Scale concentration, scale (kg/m ³)	0.0 0.2121* 0.5	735 735 735	0.19 0.19 0.18‡	-0.19 -0.19 -0.19	785 795 795
Vapor pressure lowering scale factor, bfact	0.7 0.8 0.9 1.0* 1.02 1.035 1.05 1.1 1.3	185 295 485 735 805 875 955 > 1,000 > 1,000	0.19‡ 0.19 0.19 0.19 0.19 0.19 0.19 0.19 	-0.22 -0.21 -0.20 -0.19 -0.19 -0.19 -0.19 -0.19 -0.19 -0.19	385 385 544 795 865 925 > 1,000 > 1,000 > 1,000
Initial salt, <i>dsalt</i> (kg)	0.0 0.1* 5.0	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	795 795 775

Table 4-3. Deterministic parametric study for thermal and environmental models (cont'd)

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Parameters	Parameter Values	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	t _f (yr)
Initial scale, <i>dscale</i> (kg)	0.0* 0.5 15.0	735 735 735	0.19 0.19 -0.50	-0.19 -0.19 -0.19	795 795 > 1,000
Funnel area, <i>qfrac</i> (m ²)	0.1 1.0* 10.0	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	795 795 785
Umbrella edge thickness, slice (m)	1.0 20.0* 30.0	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	785 795 795
Umbrella edge temperature, tenhan (°C)	90 95* 98	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	785 795 795
Range of umbrella edge temperature, <i>tslop</i> (°C)	0.1 2.0* 5.0	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	785 795 795
* Base case † Variation to -0.18 V _{SHE} ‡ Variation to -0.5 V _{SHE}					

Table 4-3. Deterministic parametric study for thermal and environmental models (cont'd)

1,000-yr period. Since the radioactive decay of spent fuel can be represented as a function of time by an approximately exponential decline in heat generation per unit mass of initial heavy metal in the fuel and the mass of initial heavy metal per waste package is fixed, then the amount of initial heat generated per waste package is less resulting in lower peak temperatures at the container surface. However, it will remain for longer time periods at elevated temperatures since older fuel decays more slowly. The result is understandable because an older initial age of the spent fuel at the time of emplacement requires closer spacing of the waste packages to obtain the desired initial areal thermal loading. It is interesting to note that for 10-yr age fuel with all the other input parameters representing the base case, as given in Tables 3-1 and 3-2, t_f is 795 yr indicating that the container wall was penetrated in 60 yr as a result of localized corrosion, because E_{corr} was higher than E_{crit} as soon as the container became wet after 735 yr of emplacement. For fuel with ages of 15 and 18 yr, although E_{corr} varied from -0.53 to $-0.18 V_{SHE}$, it remained for a time sufficiently long below E_{crit} . As a consequence, failure did not occur in a 1,000-yr period. For the 15-yr fuel age, it is clear that the container surface was wet for at least 255 yr without complete wall penetration.

4.2.1.2 Rock Properties

An increase in the thermal conductivity of the rock led to a decrease in the temperature difference between the canister and the rock a few meters away from the containers, as expected, shortening the period during which the container surface remained dry. As shown in Table 4-3, t_w decreased with increasing thermal conductivity and a variation of 20 percent in this parameter around the base case value altered t_w by about 18 to 25 percent. Despite the variation in the wetting time, E_{corr} remained constant at approximately 0.18 V_{SHE} because E_{corr} is not very sensitive to minor variations in temperature. On the other hand, E_{crit} increased by about 20 mV with increasing thermal conductivity mostly reflecting increases in temperature and small decreases in the chloride concentration. The overall result is a decrease in t_f from 985 to 595 yr with increasing thermal conductivity. The variation from 60 to 40 yr in the time required for full penetration of the container wall by localized corrosion is not considered significant in the present analysis.

An even larger relative variation (26 percent) of the thermal conductivity of the packing had no effect on the temperature difference between the containers and the rock, and, therefore, on the wetting time (Table 4-3). This is essentially the result of dimensional factors because the packing fills a small (about 1 cm) annular gap around each container. It appears that only a substantially larger amount of a packing material with very low thermal conductivity could produce a noticeable delay in the wetting time of the container.

The volumetric heat capacity of the rock affects the time period during which the container surface remains dry because the temperature of the repository as a whole increases with increasing heat capacity. Hence, the temperature of the containers also increases. As indicated in Table 4-3, an increase in the volumetric heat capacity from 2.0×10^6 to 3.0×10^6 J/m³/°K (50 percent increase) increased t_w monotonically from 725 to 805 yr. The corrosion potential did not change significantly with this variation of heat capacity, but the difference in temperature at the container surface, and mainly in chloride concentration, induced by this variation produced a decrease of about 30 mV in E_{crit} . The time required for container wall penetration after wetting decreases monotonically from 150 to 40–50 yr. It should be

noted that 10-yr time steps were used in this simulation, and, therefore, the distinction between 40 and 50 yr may be insignificant.

Variations over a relatively wide range in the tortuosity and porosity of the rock did not have any effect on the wetting time. These are two factors that affect the evaporation rate of water from the container surface, but no effect should be expected on the corrosion parameters as shown in Table 4-3.

4.2.1.3 Chemistry Effects

The water film thickness was varied over a reasonable range (0.1 to 4.0 mm). As expected, this variation should not affect the wetting time because this is a parameter only relevant to the diffusion of molecular oxygen, in the eventual case in which the salt scale is not formed. Nevertheless, no effect on the corrosion potential was observed over that range of variation and the minor changes shown in Table 4-3 for t_f (785 to 805 yr) are within the range expected for the time steps used in the simulation.

The salt concentration and the scale concentration did not have any effect on t_w although they were both varied over a relatively large range. However, a very large value of the salt concentration should decrease the vapor pressure enough to promote premature wetting. Similarly, no effect on the corrosion parameters was noted, as shown in Table 4-3.

A parameter that has a very important effect on the wetting time is the vapor pressure lowering scale factor that was varied from 1.0 to 0.7 to represent the effect of salts that produce a lowering in the vapor pressure of water increasingly greater than that of NaCl. As shown in Table 4-3, t_w decreased from 735 to 185 yr by decreasing this parameter from 1.0 to 0.7. On the other hand, an increase of the parameter to 1.1, corresponding to salts with vapor pressure lowering smaller than that of NaCl, led to t_w longer than 1,000 yr. The variation in this parameter produced some variation in E_{corr} that decreased from 0.199 to 0.185 V_{SHE} with increasing values of the scale factor. It should be noted, however, that E_{corr} decreased down to $-0.5 V_{SHE}$ from 0.19 V_{SHE} for a value of 0.7. Corresponding to this case, the time required for penetration of the container wall once the surface became wetted was 200 yr. This time decreased to 90 yr for a scale factor of 0.8 and became 50-60 yr for the remaining cases except when t_w was equal or greater than 955 yr. The variation of t_w and t_f with the vapor pressure lowering scale factor is clearly illustrated in Figure 4-3.

Although this parameter includes the influence of other salts besides NaCl on the vapor pressure lowering, there is not specific consideration of their chemical nature, which undoubtedly has an important effect on corrosion. Nitrate, for example, acts as an inhibitor of the localized corrosion of stainless steels by raising the critical potential in chloride-containing solutions.

The remaining parameters related to the thermal/environmental models that were varied in this sensitivity study are shown in Table 4-3. Although they were varied over a relatively large range, none of them affected t_w , which was found to be equal to 735 yr for all the cases run. No effect was observed in t_f that was always equal to 775-795 yr, with the single exception of the largest value for the initial scale. When a value of 15 kg was adopted for the initial scale, $E_{\rm corr}$ became equal to $-0.5 V_{\rm SHE}$ and since no localized corrosion initiated because that value is lower than $E_{\rm crit}$, no failure occurred during the 1,000-yr simulation period.



Figure 4-3. Effect of vapor pressure lowering scale factor on the time-to wetting and time-to-failure for baseline case (type 304L SS in uncontrolled environment)

4.2.2 Corrosion-Related Parameters

In the parametric study of corrosion-related parameters, the wetting time, as expected, was always equal to 735 yr. In addition, for the baseline case of a type 304L SS container in an uncontrolled environment, $E_{\rm crit}$ was always found to be equal to $-0.193 V_{\rm SHE}$, despite the variation in the input parameters, because its value is determined only by temperature and chloride concentration.

An increase in the transfer coefficient for the oxygen reaction (β) from 0.25 to 0.75 produced a decrease in $E_{\rm corr}$ from 0.564 to 0.188 $V_{\rm SHE}$, as shown in Table 4-4. Since any value within that range is higher than $E_{\rm crit}$, propagation of localized corrosion took place and failure, as a result of container wall penetration, occurred in 795 yr. On the other hand, a variation from 0.25 to 0.5 in the equivalent parameter for the water reduction reaction did not affect $E_{\rm corr}$ and, therefore, no effect on t_f was observed.

An increase in the rate constant for the oxygen reduction reaction (k_{O_2}) of about eight orders of magnitude increased $E_{\rm corr}$ from 0.090 to 0.286 $V_{\rm SHE}$. As in the previous case, this variation did not affect t_f because $E_{\rm corr}$ was always greater than $E_{\rm crit}$. A similar variation in the rate constant for the reduction of water did not modify $E_{\rm corr}$ and, therefore, no change in t_f occurred.

As expected, a variation of three orders of magnitude in the current density (corrosion rate) for air/steam did not affect t_f . However, if the active current density is lowered from 6.3×10^6 to 6.3×10^5 C/(yr \cdot m²), the rate of penetration, once localized corrosion initiated, decreased sufficiently to eliminate failure within the 1,000-yr simulation period. On the other hand, an increase of one order of magnitude in this rate led to failure within the year in which the container became wet. Regardless of the values adopted, the assumption of a constant active current density is conservative because in natural systems corrosion rate usually decreases with the square root of time.

The current density of the passive surface, expressed as *Cpass* coefficient, is important in determining the corrosion potential. If this dissolution rate is large enough to be comparable with the dissolution rate under active corrosion conditions rather than under typical passive conditions, $E_{\rm corr}$ may attain very low values. This happened when this parameter was increased to 6.3×10^5 C/(yr \cdot m²). In this case, as shown in Table 4-4, $E_{\rm corr}$ was found to be equal to -0.645 $V_{\rm SHE}$. Under such conditions, t_f became greater than 1,000 yr because $E_{\rm corr}$ remained lower than $E_{\rm crit}$ and localized corrosion did not initiate.

The last two parameters that may have an effect on the corrosion potential are the tortuosity factor for the scale and the scale porosity. The tortuosity factor did not have an effect on $E_{\rm corr}$ over a wide range of values (Table 4-4). Only when it attains a value of 0.05, does it produce a decrease of $E_{\rm corr}$ from 0.188 to -0.462 $V_{\rm SHE}$ In the case of the scale porosity, a value of 0.1 decreased $E_{\rm corr}$ over a 0.188 to -0.431 $V_{\rm SHE}$. Both represent cases in which the reduction of oxygen and, therefore, the corrosion potential became controlled by the diffusion of oxygen through the scale rather than by activation kinetics at the metal/scale interface. In both cases, as noted above, a decrease of $E_{\rm corr}$ below

Parameters	Parameter Values	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	<i>t_f</i> (yr)
Oxygen beta kinetics parameter, betaox	0.25 0.5 0.75*	735 735 735	0.56 0.28 0.19	-0.19 -0.19 -0.19	795 795 795
Water beta kinetics parameter, <i>betahy</i>	0.25 0.5*	735 735	0.19 0.19	-0.19 -0.19	795 795
Rate constant for oxygen reduction, <i>rkox</i> [C • m/(mole • yr)]	$3.0 \times 10^{6} \\ 3.0 \times 10^{10*} \\ 3.0 \times 10^{14}$	735 735 735	0.09 0.19 0.29	-0.19 -0.19 -0.19	795 795 795
Rate constant for water reduction, <i>rkhy</i> [C/(m ² • yr)]	$3.2 \times 10^{-4} \\ 3.2^{*} \\ 3.2 \times 10^{4}$	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	795 795 795
Current density for air/steam, curair [C/(yr • m ²)]	$ \begin{array}{r} 6.3 \\ 6.3 \times 10^{2*} \\ 6.3 \times 10^3 \end{array} $	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	795 795 795
Active current density, curact [C/(yr • m ²)]	6.3×10^{5} $6.3 \times 10^{6*}$ 6.3×10^{8}	735 735 735	0.19 0.19 0.19	-0.19 -0.19 -0.19	>1,000 795 735
Cpass coefficient aa(1) [C/(yr • ×m ²)]	$6.3 \times 10^{3} \\ 6.3 \times 10^{4*} \\ 6.3 \times 10^{5}$	735 735 735	0.21 0.19 -0.65	-0.19 -0.19 -0.19	795 795 >1,000

 Table 4-4. Deterministic sensitivity study of input parameters for corrosion models

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Parameters	Parameter Values	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	<i>t_f</i> (yr)
Tortuosity factor for scale, taus	0.05 0.3* 1.0	735 735 735	-0.46 0.19 0.19	-0.19 -0.19 -0.19	> 1,000 795 795
Scale porosity, spor	0.1 0.5* 1.0	735 735 735	-0.43 0.19 0.19	-0.19 -0.19 -0.19	>1,000 795 785
 * Base case † Variation to -0.18 V_{SHE} ‡ Variation to -0.5 V_{SHE} 				<u> </u>	

 Table 4-4. Deterministic sensitivity study of input parameters for corrosion models (cont'd)

the value of E_{crit} eliminated the initiation of localized corrosion and, therefore, t_f became greater than 1,000 yr, even though the container was wet after 735 yr of emplacement.

4.3 ALTERNATIVE CONTAINER MATERIAL AND ENVIRONMENT CASES

As summarized in Tables 2-1 and 2-2, several test runs of the SCCEX code were conducted for evaluating the failure time of several alternative container materials under different environmental conditions. In the first set of these tests, the results summarized in Table 4-5 for a 10-yr age fuel were obtained. The results for type 304L SS as a container material in an uncontrolled environment, resulting from the evaporation and concentration of the groundwater, were already discussed as the baseline case but are included in the table for comparison. Regardless of the container material and the differences in the chloride concentration of the environment, t_w was equal to 735 yr in all cases. Considering the influence on container life of the degradation processes that occurred after wetting, the use of alloy 825 as a container material (Alt-1) did not modify t_r , which was identical to that obtained for type 304L SS. Although E_{crit} for alloy 825 in the highly concentrated chloride environment is 70 mV higher than that for type 304L SS, such a difference did not introduce any change in the time required for wall penetration because E_{corr} was sufficiently high to promote localized corrosion in both materials. An identical t_f was obtained for type 304L SS in the controlled chloride environment (Alt-3), despite the fact that E_{crit} was displaced to $-0.043 V_{SHE}$ in the presence of a low chloride concentration. However, this modification in the composition of the environment avoided the occurrence of localized corrosion in the case of alloy 825 (Alt-4) because E_{crit} was higher than E_{corr} . As a consequence, no failure occurred in the 1,000-yr period of simulation for this case.

For the alternative material X, a relatively high passive current density of 1.26×10^{6} C/(yr · m²), coupled with a relatively high value of 0.8 V_{SHE} for E_{crit} , was assumed in order to define a corrosionallowance material. It should be noted that E_{corr} had a very low value, as expected for a material with low resistance to general corrosion since it does not exhibit passive behavior. In this particular case (Alt-4), t_f reached 970 yr and failure was due to buckling as a result of the collapse of the container walls once the wall thickness decreased to a very low value (0.15 cm) by generalized corrosion. By increasing the wall thickness to 2 cm, t_w became equal to 743 yr, which is a value similar to that found in all the other cases shown in Table 4-5. It is apparent that doubling the wall thickness has no effect on the thermal and environmental variables affecting the wetting of the container. However, t_f increased to 1,200 yr as a result of the additional time required to reduce the wall thickness to a value at which buckling predominated.

In the following case (Alt-5), failure due to stress corrosion of the alternative material Y occurred after 780 yr. Crack propagation leading to failure occurred after a 20-yr initiation period because $E_{\rm corr}$ lay within the potential range, defined by E_{rp} and E_{p} , in which Y is susceptible to stress corrosion cracking in chloride-containing solutions.

In the Alt-6 case, in which Z was used as container material, no failure occurred in the 1,000-yr period, although the container became wet after 735 yr. The value of $E_{\rm corr}$, as shown in Table 4-5, was significantly lower than $E_{\rm crit}$ and, therefore, no localized corrosion occurred. This is a material with a very low passive current and, therefore, resistant to general corrosion.

Case	Material	Environment	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	t _f (yr)	Temp. at 1,000 yr (°C)
Baseline	Type 304L SS	Uncontrolled Cl concentration. Intermediate thermal power density.	735	0.18	-0.19	795	91.9
Alt-1	Alloy 825	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	735	0.18	-0.12	795	91.9
Alt-2	Type 304L SS	Controlled Cl ⁻ (< 100 ppm) concentration. Intermediate thermal power density.	735	0.18	-0.04	795	91.9
Alt-3	Alloy 825	Controlled Cl ⁻ (< 100 ppm) concentration. Intermediate thermal power density.	735	0.18	0.22	>1,000	91.9
Alt-4	x	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	735	-0.71	0.80	970	91.9
Alt-5	Y	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	735	0.18	0.09 to 0.58	780	91.9
Alt-6	Z	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	735	0.18	0.80	>1,000	91.9

Table 4-5. Results of example problem test cases for 10-yr fuel

Table 4-6 includes additional alternative test cases for 30-yr age fuel. These test runs were performed for the purpose of further comparison with some of the results of the probabilistic analyses. No wetting was observed in the 1,000-yr period, and, therefore, no failure due to corrosion-related processes was observed. The materials involved, type 304L SS (Baseline-A), alloy 825 (Alt-3-A), and Z (Alt-6-A and Alt-6-B), are all characterized by their excellent mechanical properties in terms of yield strength and fracture toughness, and, therefore, they were not prone to mechanical failures by buckling, yielding, or fracture.

Case	Material	Environment	t _w (yr)	E _{corr} (V _{SHE})	E _{crit} (V _{SHE})	t _f (yr)	Temp. at 1,000 yr (°C)
Baseline-A	Type 304L SS	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	>1000	_	—	> 1,000	119.0
Alt-3-A	Alloy 825	Controlled Cl ⁻ (< 100 ppm) concentration. Intermediate thermal power density.	> 1000	_	_	> 1,000	119.0
Alt-6-A	Z	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	>1000			>1,000	119.0
Alt-6-B	Z	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	> 1000			> 1,000	119.0

 Table 4-6. Results of example problem alternative test cases for 30-yr fuel

5 SYSTEM CODE ANALYSES

The SCCEX deterministic code has been integrated with the total system performance assessment (TPA) code and executed via a driver code named SMLEXC. The SMLEXC code uses the LHS method to generate sampling vectors for the defined random variables listed in Tables 3.1 and 3.2. The SCCEX deterministic code is then repeatedly run for each sampled LHS vector.

Because of the constraints in analysis time and computer resources, only 100 LHS vectors were used in the SCCEX probabilistic analyses. In addition, it was necessary to assume that the waste packages can be represented by a reasonably small number of cells, where each cell has multiple waste packages subject to identical environmental conditions. In the example problem, 256 cells were used to model all the 30,000 waste packages. As a result of the one-eighth symmetry of the problem, only 36 cells need to be modeled, as shown in Figure 2-2. In this way, groups of four or eight cells, subjected to identical environmental conditions, are defined depending on their location, either along the diagonals or in any other position of the modeled repository. The grouping simplification was made so that for each generated LHS vector, calculations are only required for 36 cells, rather than for about 30,000 waste packages. By using a probabilistic global/local analysis approach described in Section 5.3, the validity of the grouping assumption can be checked and the model can be improved when found necessary. A larger number of LHS simulations may be necessary if high resolution is required for a small number of waste package failures. In the extreme case, each waste package could have a different life, as defined by the failure time, because of the differences in local environmental conditions, geometry, fabrication defects, fuel contents, etc. As discussed in Section 5.4, further improvements can be made.

In the system code, life calculations are performed sequentially for each group assuming no interactions between the groups. The time-to-failure results associated with cells are stored in an output file. The data can be processed using the post-processing code, POST, which generates empirical CDF and PDF data for three types of plots.

The empirical CDF is generated using the equation CDF = (i - 0.5)/N where *i* is the ordered number of the failures (from 1 to N) and N is the total number of simulations. The PDF is computed by counting the numbers of failure within different time increments (i.e., bins).

In developing the example problem, the same probabilistic analysis procedure was repeated for five different materials under various environmental conditions, as summarized in Tables 2-1 and 2-2. The probabilistic analysis results will be illustrated using type 304L SS as container material under controlled environmental conditions (Alt-2) and material Z under uncontrolled environmental conditions (Alt-6), as shown in Table 2-1.

5.1 PROBABILISTIC ANALYSIS PROCEDURE AND RESULTS

One of the three types of plots shows the CDF of time-to-failure for the *worst group*, which is defined as the group with the lowest average life in 100 simulations. Because a group typically contains several hundred waste packages, the worst group CDF provides an indication of the minimum waste package containment capability. If the reliability of the worst group does not meet the SCC requirement, then it would not be necessary to do a detailed analysis of all the groups. On the other hand, if the reliability of the worst group is acceptable, more detailed analyses may be needed to focus on the local variations within a group. The CDF result for the Alt-2 case is shown in Figure 5-1. This figure shows



Figure 5-1. Time-to-failure CDF for the worst group of cells corresponding to Alt-2 case (type 304L SS in controlled chloride environment)

that the probability is greater than 50 percent that the worst cell will fail before 1,000 yr. The CDF results are approximate, as reflected by the unevenness of the curves that can be attributed to the insufficient sampling (only 100 LHS vectors).

The second plot is a CDF plot for several selected cumulative numbers of cell failures. This plot is useful for examining the reliability of a group (or translated into waste packages) for the selected number of failures, at a selected time. For example, it can give the result on the probability that a quarter (i.e., 64) of the total cells will fail before 1,000 yr. The result for the Alt-2 case is shown in Figure 5-2. CDFs for three cumulative numbers of cell failures are plotted. The plot indicates that there is about a 10-percent probability that all the cells will fail before 1,000 yr.

The third plot is a PDF of the number of cell failures, which can be translated into the number of waste package failures. This plot shows the probability of failure at several selected times. The results for the Alt-2 case are shown in Figure 5-3 for 300, 650, and 1,000 yr. It shows that the reliability of zero failures decreases significantly as a function of time. The probability of zero failures is 0.87 at 300 yr and drops to 0.45 at 1,000 yr. The figure also shows the trend of probability increasing for total (all 256 cells) failures. The probability of total failures should approach 1 as time increases. The PDF plot is a useful way to quantitatively present the SCC analysis in probability terms.

The three plots for the case of material Z (Alt-6) are shown in Figures 5-4 to 5-6. By comparing these figures with those for type 304L SS (Alt-2 case), it is apparent that a material with more resistance to localized corrosion exhibited a significantly lower CDF value at any given failure time, and the PDF values are concentrated at the zero number of failed cells.

Figure 5-7 compares the CDF of the worst group of cells for the baseline case of a type 304L SS container under uncontrolled environmental conditions assuming low, intermediate, and high thermal power densities. In this analysis, only the high thermal power density condition produces a decrease in the CDF values with respect to those at lower thermal power densities. However, no significant effect on the thermal loading on the CDF values is noted, especially at extended failure times (> 600 yr).

Figure 5-8 compares the CDF for the worst group of cells for the complete set of cases included in Table 2-1. All the cases included are for intermediate thermal power density. The plot clearly revealed the differences between the various cases and, in particular, the significant improvement exhibited in the Alt-6 case. It is apparent that this methodology can be used to distinguish various materials and design options quantitatively.

5.2 EXAMPLE OF A PROBABILISTIC SUBSTANTIALLY COMPLETE CONTAINMENT RULE

In general, a probabilistic interpretation for the SCC rule could involve a reliability requirement for a specified number of waste package failures. For example, an example framework investigated earlier by the CNWRA and the NRC had the following SCC reliability format:

"The probability that the proportion K of waste packages failing during the period $[0, t_o]$ being less than or equal to K_o should be greater than or equal to p_o ."


Figure 5-2. CDF for selected cumulative number of cell failures corresponding to Alt-2 case



Figure 5-3. PDF of the number of cell failures at selected times corresponding to Alt-2 case



Figure 5-4. Time-to-failure CDF for the worst group of cells corresponding to Alt-6 case (material Z in uncontrolled environment)



Figure 5-5. CDF for selected cumulative number of cell failures corresponding to Alt-6 case



Figure 5-6. PDF of the number of cell failures at selected times corresponding to Alt-6 case



Figure 5-7. Time-to-failure CDF for the worst group of cells in the baseline case (type 304L SS in uncontrolled environment) at low, intermediate, and high thermal power density

5-9



Figure 5-8. Time-to-failure CDF for the worst group of cells in the baseline case and the six alternative cases given in Table 2-1 at intermediate thermal power density

In symbols,

$$\operatorname{Prob}\left\{K \leq K_{o}\right\} \geq p_{o} \tag{5-1}$$

where K is the proportion of waste packages failing in time, t_o , and p_o , called the reliability target, is the minimum acceptable probability that $K \leq K_o$. This example framework, as well as the method to deal with the uncertainty in demonstrating the above requirements was presented in a NUREG report. (Wu et al., 1991).

The previous probabilistic analyses results, which are based on cells, each including a large number of waste packages, may not provide sufficient details required by such a SCC rule. To compute probabilistic solutions based on a small number of waste packages, the following global/local approach can be used.

5.3 A PROBABILISTIC GLOBAL/LOCAL ANALYSIS APPROACH

Current analyses use only 100 samples which are insufficient for investigating SCC at the low probability of failure region (i.e., less than 0.01). Furthermore, the grouping approach disregards the variabilities among the waste packages in the same group. However, these global analyses can provide valuable information on the general deterministic and probabilistic behaviors of the waste packages. For example, the results identified the weakest spots (i.e., the corner cells tend to fail first because the corners are cooler and get wet first). The results also suggested that mechanical failures are secondary failure modes in comparison with corrosion-induced failures.

Based on the results of the complete but coarse (global) model, more refined and focused (local) analyses can be performed in a more efficient manner by applying an importance sampling method. Selective local sampling is applied to the cells more likely to fail under more unfavorable input conditions. This approach is called probabilistic global/local analysis.

There are several ways to define the worst group. The one used here is based on the total number of times the group fails in 100 simulations. It is important to know the other weak groups. The POST program calculates the number of times each group failed first, second, . . . etc. This information is useful to define the worst groups.

Once the weakest cells have been identified, local analyses can focus on these cells where the waste packages might fail before 1,000 yr. Figure 5-9 shows a model for a local analysis for the use of material Z (Alt-6). By focusing on a small fraction of the total cells and thus saving the analyses time, it becomes practical to introduce waste package variabilities within a cell to develop a more refined SCC evaluation. In other words, different waste packages within a cell could fail at different times due to, among other factors, local variations in temperature, fabrication defects, and geometry differences.

The global analysis for Alt-6 indicated that the four corner cells failed 93 out of 100 times. A local analysis was performed at one of the four corners. The corner has 512 waste packages that are modeled separately. In this analysis, the only variable which exhibits differences among the waste packages is temperature, but the analysis can be extended to other factors if needed. Changes in the heat load within the repository and/or change in material performance in the given environment will alter the locations of the worst cells. The CDF for selected total number of waste packages are plotted in



Note: A = 4 cells, B = 8 cells (1/8 model)

Figure 5-9. Schematic diagram of the model for the local analysis of the corner cells

Figure 5-10, which clearly shows the local variability within the corner. The PDF of the waste packages, using the ratio K as the unit, is shown in Figure 5-11. This shows that the local analysis can provide calculational results with a level of detail that can evaluate a small number of container failures. The local analysis is limited, however, by how detailed local variations in environmental parameters and other factors can be modeled.

In general, the local analysis should be applied to cover sufficient adjacent cells of the worst group to avoid missing weak waste packages. An adaptive approach can be devised to gradually increase the analysis zone around the worst group until the increased zone does not change the waste package PDF in the SCC region of interests.

In the case where there is randomness within a cell, importance sampling can be applied to the input probability distributions to limit the parameter sampling space such that the generated samples will produce shorter (less than 1,000 yr) waste package lives. The adaptive importance sampling method which adaptively adjusts and determines an optimal sampling space can be used for efficient, small probability failure analyses. This approach was also discussed in the previous SCC methodology investigation report (Wu et al., 1991).

5.4 ALTERNATIVE CONTAINER MATERIAL AND ENVIRONMENT CASES

The results of all the cases studied using probabilistic analyses are summarized in Tables 5-1 and 5-2. The results are expressed in terms of the percentage of cells that became wet and failed before the end of the simulation for both 300- and 1,000-yr periods.

For the baseline case of type 304L SS container in uncontrolled environmental conditions, an increase in the initial thermal power density of the repository decreased the percentage of cells (waste packages) that became wet after both 300 and 1,000 yr. The percentage of failed waste packages also decreased with increasing thermal loading. Contrary to the findings of the deterministic analysis in which a minimum time-to-wetting and a minimum time-to-failure was calculated at intermediate thermal power density, in this case, the percentage of cells that became wet and failed for both 300- and 1000-yr periods decreases monotonically with increasing thermal power density.

For all the cases summarized in Table 5-1, corresponding to the intermediate thermal power density, the percentages of waste packages wetted after 300 and 1,000 yr were found to be equal to 3.2 and 29.6 percent, respectively. However, the percentage of failed packages is strongly dependent on the material and the environmental conditions defined for each case. The use of alloy 825 (Alt-1) only represents a minor improvement with respect to type 304L SS, but a substantial reduction in the percentage of failed containers is obtained under controlled environmental conditions (Alt-3). In the case of type 304L SS containers (Alt-2), this controlled environment has no beneficial effect.

By comparing the remaining cases in Table 5-1, it is apparent that the use of material Z (Alt-6) represents a significant improvement in performance because the percentage of failed packages decreased to 0.0 after 300 yr and to 4.4 after 1,000 yr. On the other hand, although both materials X (Alt-4) and Y (Alt-5) exhibited very good performance after 300 yr of emplacement, the percentage of failed packages increased substantially in the 1,000-yr period. For the Alt-4 case the percentage increased from 0.0 to 12.5, but for the Alt-5 case, the increase from 0.69 to 17.1 is even more noticeable.



Figure 5-10. CDF for selected cumulative number of waste package failures in the corner cell corresponding to Alt-6 case



Figure 5-11. PDF at selected times for waste package failures in the corner cell corresponding to Alt-6 case

Table 5-1. Results of probabilistic SCCEX code test runs

				300 yr		1,000 yr	
Cases	Material	Environment	Random Variable Ranges	Wetted (%)	Failed (%)	Wetted (%)	Failed (%)
Baseline-H	Type 304L SS	Uncontrolled Cl ⁻ concentration. High thermal power density.	Baseline	0.37	0.093	9.45	7.23
Baseline-I	Type 304L SS	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	Baseline	3.18	2.0	29.56	22.40
Baseline-L	Type 304L SS	Uncontrolled Cl ⁻ concentration. Low thermal power density.	Baseline	15.4	12.4	57.6	50.36
Alt-1	Alloy 825	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	Baseline	3.18	1.07	29.56	18.44
Alt-2	Type 304L SS	Controlled Cl ⁻ (<100 ppm) concentration. Intermediate thermal power density.	Baseline	3.18	1.07	29.56	18.28
Alt-3	Alloy 825	Controlled Cl ⁻ (< 100 ppm) concentration. Intermediate thermal power density.	Baseline	3.18	0.03	29.56	9.08
Alt-4	x	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	Baseline, Cpass range $(1.2-1.3 \times 10^6)$	3.18 0		29.56	12.47
Alt-5	Y	Uncontrolled Cl concentration. Intermediate thermal power density.	Baseline	3.18	0.59	29.56	17.09
Alt-6	Z	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	Baseline	3.18	0.0	29.56	4.41

				300 yr		1,000 yr	
Cases	Material	Environment	Random Variable Ranges	Wetted (%)	Failed (%)	Wetted (%)	Failed (%)
Baseline-A	Type 304L SS	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	Modified	3.89	0.39	28.55	15.05
Alt-3-A	Alloy 825	Controlled Cl ⁻ (<100 ppm) concentration. Intermediate thermal power density.	Modified Cpass range $(6.3 \times 10^3 - 6.3 \times 10^4)$	3.89	0.00	28.55	0.84
Alt-6-A	Z	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	Modified	3.89	0.00	28.55	4.03
Alt-6-B	Z	Uncontrolled Cl ⁻ concentration. Intermediate thermal power density.	Modified Cpass range $(6.3 \times 10^3 - 6.3 \times 10^4)$	3.89	0.00	28.55	0.00

Table 5-2. Results of probabilistic SCCEX code test runs for additional alternative cases

The tests cases summarized in Table 5-2 correspond to packages containing 30-yr age fuel emplaced in a repository at an intermediate thermal power density. In all of these cases, the percentage of wetted packages increased from 3.9 to 28.6 in the time interval between 300 and 1,000 yr. The percentage of failed packages at 300 yr was found to be zero with the exception of the Baseline-A case in which 0.39 percent of the packages failed. However, it is very important to note that at 1,000 yr, a certain proportion of packages did fail. These results should be compared with the results of the deterministic analyses summarized in Table 4-6. Whereas the deterministic analyses showed that no wetting or failure occurred in a 1,000-yr period, the probabilistic analyses clearly indicated that a relatively large percentage of packages failed in the different cases (Baseline-A, Alt-3-A, and Alt-6-A) with the exception of the Alt-6-B case, in which the percentage is zero.

6 SUMMARY AND CONCLUSIONS

As part of the calculations conducted in the example problem for the "substantially complete containment" rule for waste packages, both deterministic and probabilistic analyses were performed. The calculations provide a valuable insight into the nature of the interdependence between the thermal, environmental, corrosion, and mechanical models, as well as on the influence and importance of the parameters associated with each type of model. The most significant aspects of the results obtained in these analyses and an evaluation of the methodology adopted in this study are discussed below.

6.1 **RESULTS OF THE DETERMINISTIC AND PROBABILISTIC STUDY**

The parametric study of the effect of initial thermal power density on the time-to-failure of the waste package clearly reveals the significance of the period during which the container remains dry on the overall life of the container. The time-to-wetting was found to be a complex function of the initial thermal power density exhibiting a minimum at intermediate power densities, just above the value selected in the SCP for the current thermal loading strategy. At higher thermal power densities, a significant increase in the wetting time was noted-a 12 percent increase in the thermal power density led to an increase of approximately 40 percent in the wetting time. It should be noted that a high thermal loading strategy implies, at least, the doubling of the thermal power density currently considered. The wetting time rather than the time required to breach the container by localized corrosion is the predominant component of the overall life of the container for the waste package used in this study as a baseline case, which is the reference design in the SCP with type 304L SS as container material. In this case, the time required for the penetration of the container wall by localized corrosion represents, at the most, 30 percent of the total time-to-failure for all the range of thermal power densities covered in the parametric study. However, for alloy 825 as container material and a controlled environment characterized by a relatively low chloride concentration, the time during which the container remains wet but without penetration by localized corrosion increases substantially.

The deterministic study of other thermal and environmental parameters reveals that few of them, within the range of variation examined, influence the time-to-wetting. The wetting time is increased by increasing the age of the fuel, the volumetric heat capacity of the rock, and the vapor pressure lowering scale factor. On the other hand, the wetting time decreases by increasing the thermal conductivity of the rock. Although, as a result of the small dimensions of the annular gap filled with packing material, no effect of the thermal conductivity of the packing was found, it can be concluded from the analysis that a backfill material with a very low thermal conductivity may delay significantly the wetting of the container. Other parameters for the thermal model related to the properties of the rock, such as the tortuosity and the porosity, appear to have insignificant effect to the wetting time.

The vapor pressure lowering scale factor, as expected from the conceptual modeling of the nearfield environment model, has a dominant effect on the wetting time. Salts with a higher solubility in water than that of NaCl, such as NaNO₃ and CaCl₂, which are characterized by a vapor pressure lowering scale factor lower than 1.0, can promote the formation of a liquid film on the container surface much faster than NaCl, which is the salt of reference in the environmental model. On the contrary, the presence on the container surface of a salt which is less soluble in water than NaCl, such as Na₂CO₃, leads to a longer time-to-wetting. Other parameters incorporated in the environment model, such as the water film thickness, the salt concentration, the scale concentration, and the initial amount of salt or scale present in the container surface, do not affect the wetting time. No effect on the time-to-wetting was also found for the parameters characterizing the hydrothermal umbrella.

The factors affecting the life of the waste package, as defined by the time-to-failure of the containers, can be classified in two groups. One group consists of all the parameters that modified the wetting time as noted above and, therefore, they indirectly affect the failure time. The other group includes all the parameters that have an intrinsic effect on the corrosion process. Within this group of parameters, an increase in the transfer coefficient for the oxygen reduction reaction (oxygen beta kinetic parameter), as well as a decrease in the rate constant for the oxygen reaction, promotes a gradual decrease in the corrosion potential by altering the kinetics of the charge transfer reaction. A more abrupt decrease in the corrosion potential is found when the transport of oxygen to the metal solution interface is retarded by the presence of a scale formed on the container surface. Very low corrosion potentials, corresponding to reducing conditions, were found to be associated with very low values for the tortuosity factor and the porosity of the scale.

The value of the passive current density also alters the corrosion potential. The corrosion potential decreases gradually with increasing passive current density. However, an abrupt decrease of the corrosion potential to very negative values (reducing conditions) is attained at relatively high current densities, typical of actively corroding metals. As clearly indicated by some results of the parametric study, a decrease in the corrosion potential can significantly increase the life of the waste package because the critical potential for the occurrence of localized corrosion is not reached under the environmental conditions established at the container surface. On the other hand, if the corrosion potential is higher than the critical potential for the occurrence of localized corrosion, the results of the parametric calculations show that the value of the active current density accounting for the metal dissolution rate at the bottom of a pit or any other localized corrosion area will determine, as expected, the failure time. A conservative approach has been adopted in the analysis by assuming a constant penetration rate. Many metals exhibit a corrosion. It was shown in the parametric study that the failure time increases from 795 yr to well beyond 1,000 yr by decreasing the active current density one order of magnitude with respect to the baseline case.

The probabilistic analyses performed provides information on the probability of the failure of any cell within the repository in less than a defined period of time. For the case of the type 304L SS container material exposed to a moderate chloride environment, it was shown that the probability of failure of the worst cell before 1,000 yr was greater than 50 percent. In this case, the dominant factor is the earliest wetting time of the containers in the corners of the repository where the calculated temperatures are lower. Also in this case, the contribution from the corrosion life (i.e., the period the canister is penetrated by corrosion after wetting has taken place) to the overall failure of the cell is not significant. However, if an alternate material and/or design that modifies the critical potentials and the corrosion potential is used, the dominance of the temperature and other environmental conditions in the calculated failure times and the associated probabilities will be less.

In the case of multiple cell failures, it is noted that for a type 304L SS container material (Alt-2), there is a finite probability (greater than 5 percent) that all the cells in the repository would fail in less than 1,000 yr. This is mainly due to the early wetting of containers at the outer edges of the repository. For this case, it implies that maintaining a high heat load alone may not be sufficient to prevent failures in less than 1,000 years.

The PDF analyses for Alt-2 and Alt-6 cases present important results about the ability to obtain a high reliability for "zero" failures for any specified containment time requirement. In the case of Alt-2, the reliability at 300 yr is less than 90 percent, while for Alt-6, where a material with superior corrosion resistance is chosen, the reliability is nearly 100 percent. However, the probabilities for both cases drop off significantly for the 1,000-yr period. It appears that the probability values may be increased by using alternate design concepts where local near-field environments can be better controlled.

The results of the study of the different cases of alternate container materials and environmental conditions indicate that once wetting occurs, the waste package tends to fail rapidly. The failure time can be extended by:

- (i) Choice of materials. Using materials with a higher critical potential for localized corrosion.
- (ii) Choice of design. The use of a steel overpack can lead to a significant decrease in the corrosion potential of the corrosion-resistant alloy due to a beneficial galvanic effect as soon as penetration of the overpack occurs.
- (iii) Modification of the environment. The control of the chloride concentration by appropriate backfill materials or the presence of inhibiting species, such as nitrate, can lead to increases in the critical potentials above the corrosion potential, avoiding the occurrence of localized corrosion.

Conversely, the approach adopted in this example problem allows the evaluation of different materials and conceptual designs for the waste package, ensuring that an appropriate assessment of the performance requirements is achievable.

6.2 EVALUATION OF THE METHODOLOGY

A method for evaluating the containment characteristics of waste packages over extended periods of time in a geologic repository, currently under development, is presented in this report using an example problem. The conceptual design of the waste package used in the analysis is the thin-shell container, vertically emplaced in an oversized borehole, as described in the SCP (U.S. Department of Energy, 1989). The repository is considered to be located in the unsaturated zone, and the approach for modeling the environment in contact with the waste packages is based on drip/dry concepts. In the SCCEX code, corrosion of the waste package and the corrosion potential of the material exceeds the critical potential for localized corrosion. The methodology can be used for assessing the performance of alternate waste package materials and designs, and it can be applied to saturated conditions. In the case of a saturated repository site, liquid water is present in the vicinity of the waste package at all times, and the chemical composition of the groundwater needs to be considered for evaluating the waste package performance.

Wetness of the containers is shown to be an important phenomenon in an unsaturated site, and the time-to-wetting may constitute the major portion of the life of waste packages made of materials with poor resistance to localized corrosion in concentrated chloride solutions. In future model development activities, the drip/dry model should incorporate additional mechanisms of water transport in the waste package vicinity, such as capillary flow or water migration due to heat pipe effects. Including other mechanisms will provide a better understanding of the competing processes that determine the chemical composition of the near-field environment.

In the deterministic calculations where the thermal loading for the repository was varied, it was noted that the time-to-wetting and, hence, the time-to-failure of the waste package exhibits a minimum at intermediate power densities. This behavior, if found to be well-grounded after evaluating alternate models for drip/dry processes, may have an important bearing on how the repository thermal loading strategy should be planned. It is recommended that evaluation of drip/dry models be conducted by performing carefully planned experiments that can demonstrate the validity of the critical aspects of these models.

Assuming that no event of catastrophic nature, such as volcanic activity, occurs at the repository site, the long-term integrity of the waste package is mainly dependent on the occurrence of corrosion processes caused by the presence of a liquid environment in the near field and far less dependent on the processes considered for mechanical failure. This indicates that the focus of test data collection should be on the long-term behavior of materials in appropriate near-field environments. In most cases analyzed, the final failure was controlled by localized corrosion conditions. Mechanical failures were determined to occur only when corrosion considerably degraded the load bearing capabilities of the container walls. The mechanical models used were simplified to permit the use of analytical models available in the literature. This resulted in the examination of gross section failures for the waste package and did not include any local failure conditions. In the future, local stress effects for the waste package should be modeled in detail to study local instability conditions. Additionally, processes such as microbially influenced corrosion were not considered due to the lack of suitable data. Although stress corrosion was examined, the analysis was limited by the availability of relevant data.

The deterministic analyses show how calculations can be carried out for the various failure modes considered important for the selected material and waste package design. From a regulatory perspective, such calculations should have to demonstrate that the design lifetimes equal or exceed the required containment time. In the example problem parametric variation studies were conducted. It was seen that the intuitive notion of what ranges or values of parameters are conservative could be misleading. This was seen in the deterministic study of the effect of thermal loading of the repository on the wetting time of the containers. In a multi-component analysis, where several models of varying complexities interact, the results from a deterministic analysis may not be sufficient.

The probabilistic analyses performed for the various alternative cases are useful for providing insights on how waste packages fail for ranges of parametric values. Ideally, the analyses should be conducted for each waste package as a cell and should exercise a significantly larger number of LHS simulations than those used here. However, computer cost and time for such analyses is currently prohibitive. The approach adopted in the example problem to follow a two-step calculation process appears attractive. Here, the first run is performed on a fewer number of cells (i.e., each cell contains 100 to 200 waste packages). Based on the CDF calculations, in which all cells are assumed to be independent of each other, a worst cell with the largest CDF at the earliest time-to-failure is chosen. If the CDF and the time-to-failure is not within prescribed requirements, the waste package design is deemed unacceptable. Once the waste package design is within the range of the prescribed criteria, the next level of analysis is pursued. Based on the selected worst cell, a second level LHS simulation is performed for the worst cell. The worst cell is now considered to be the domain where each of the waste packages in the worst cell is, by itself, a new cell. In this second level analysis, previously averaged

values of parameters (e.g., temperature) are replaced by the individual waste package values and may include any additional variability not previously considered, resulting, for example, from fabrication processes such as flaws or other defects. The two-step approach can provide calculated information on individual or a small number of packages. This approach may not work if many cells with a shorter life tend to fail at the same time, such that the selection of a worst cell in the first level analysis becomes impractical. To evaluate for SCC, it may be necessary to analyze the life of individual waste packages and also determine the probability that only a small number of the packages fail before the design life. Therefore, it would be necessary to adopt numerically efficient methodologies that can represent the failure probabilities for single and multiple waste packages.

The ranges of the parameters used in the example problem have been selected from the available literature and information generated at the CNWRA. In the future, new data and additional research may modify the data set used. In describing the distributions for many model parameters, uniform distributions have been assumed, with the exception of a few parameters in which a log uniform distribution was used. Other types of distributions may be more appropriate, if and when sufficient data become available. The shape of distributions may substantially alter the results of the probabilistic calculations. Nevertheless, the methodology presented in the analysis of this example problem of a reference container appears to be a robust approach for evaluating waste package lifetimes in a geologic repository.

6.3 IMPLICATIONS FOR INTERPRETATION OF SUBSTANTIALLY COMPLETE CONTAINMENT

A reliability-based interpretation of the Substantially Complete Containment regulatory requirement, like the one stated in Section 5.2, will require that a threshold value of waste package failures, K_o , and the associated probability, p_o , be specified. Any values for K_o and p_o must satisfy NRC's underlying rationale for the subsystem performance requirement which is that these must lead to added confidence in the safety of the repository, even if this increase in confidence is of a qualitative nature.

The example analyses presented in this report can be improved when design and site characterization data becomes available and as better mechanistic understanding of the various processes is achieved through further research. However, from this example, it is clear that the mechanics for probabilistic calculations exists; although its computational efficiency for accommodating a larger number of realizations and techniques for accomplishing a finer space discretization needs further work. Therefore, the estimation of reliability of the engineered barriers is certainly possible. Although this analysis was presented in the format of a performance assessment, it is to be noted that this type of analysis is equally viable for the design of the waste package. That is, once the uncertainties in the near-field environment and the material properties are known, probabilistic methods can be used to design the engineered barriers to a desired reliability level.

However, this analysis does not provide any guidance on the selection of values for K_o and p_o . If it is accepted that a probabilistic method can be adopted for the design of the engineered barriers, as argued above, then an obvious choice is, $K_o = 0$ and $p_o = 1$, which turns the reliability statement into a deterministic statement. Such extreme values of K_o and p_o are achievable to the extent the designers: (i) know the uncertainty in the environment and the material properties; (ii) have flexibility in the choice of design options (e.g., heat load, material type, emplacement configuration, etc.); (iii) adopt a probabilistic design method; and (iv) select a suitable containment period (300 to 1,000 years or other as stipulated by the Commission). Even with this obvious choice of K_o and p_o and the SCC interpreted as a deterministic statement, the NRC should choose to ask the U.S. Department of Energy to provide a reliability analysis in their license application.

In conclusion, as stated in 10 CFR 60.113, the SCC requirement may be interpreted in a deterministic manner and deemed to have no 'regulatory uncertainty,'—only 'technical uncertainties.' The technical uncertainties are related primarily to the mechanistic understanding of processes and definition of uncertainties in the near-field environment. This report should be considered as the first step in the exploration of such technical uncertainties.

7 REFERENCES

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APPENDIX A SCCEX CODE DESCRIPTION

SCCEX CODE DESCRIPTION

Substantially Complete Containment EXample (SCCEX) code is written in standard FORTRAN 77 with real*8 variables. Data are read in from an input deck and written to several output files (simple, main, summary, mechanical). Brine.f is the main program which controls the flow of all calculations. Subroutines are in files: input.f, lsodes.f, ode.f, and subroutines.f. In addition, some common blocks are stored in files: bulk.f, ecorr.f, hist.f, solve.f, vapor.f, and watt.f. The functions of these files are listed as follows:

Name	Function			
brine.f	control the flow of all calculations			
input.f	read in data from Unix standard input format			
lsodes.f	solver packages for ordinary differential equations			
ode.f	solver packages for ordinary differential equations from numerical recipes			
subroutines.f	main subroutines (include corrosion) of the program			
ecorr.f	corrosion potential variables			
hist.f	time history variables and number of print time steps			
solve.f	variables pertinent to numerical solvers			
vapor.f	vapor pressure information			
watt.f	thermal loading data			
bulk.f	common block for variables that do not fit in the other common blocks			

The approach used in the code is that data that do not generally change are preferably put in Block Data or Parameter statements. This reduces the potential for errors in the input deck. Expected units and variable definitions are included in all the common block files.

The SCCEX code follows a simple linear flow pattern as shown in Figure 2-1. First, the input file is read. Next, a series of loops are set up over the active cells, based on an assumption of symmetry of the repository area. Therefore, the input total number of cells must be a power of four.

Inside the loop over each cell lies a number of computational segments which are listed as follows:

- (i) Calculate the average repository temperature as a function of time using a convolution integral with a Green's function solution to the conduction equation.
- (ii) Calculate the difference in temperature between the container and the rock at a distance specified as an input parameter. In addition, the evaporation rate of pure water from the

container surface (i.e., evaporation assuming the container is always covered with pure water) is calculated for placing predicted evaporation rates in perspective.

- (iii) Solve a system of ordinary differential equation for
 - Volume of water on container surface (m³)
 - Mass of salts on container surface (kg)
 - Depth of corrosion (m)
 - Volume of effluent water leaving container (m^3)
 - Mass of scale on container (kg)

This step is the most computationally intensive portion of the code.

- (iv) Estimate the release rate for a single radionuclide. The radionuclide is assumed to be highly soluble. Three differential equations are solved: (a) the proportion of the initial inventory of the radionuclide remaining in the waste, (b) the proportion of the initial inventory in the waste package water, and (c) the proportion of the initial inventory released from the waste package.
- (v) Estimate the salinity inside a failed waste container assuming vapor/liquid equilibrium.

Due to the nature of the example problem, as related to containment, the release rate of radionuclides and the salinity inside a failed container are not discussed in this report despite the code has the capability to perform the computations described in (iv) and (v).

APPENDIX B EXAMPLE OF INPUT AND OUTPUT FILES FOR SCCEX CODE

EXAMPLE OF INPUT AND OUTPUT FILES FOR SCCEX CODE

As discussed in Section 2, the SCCEX code followed the flow diagram shown in Figure 2-1. The required data are: (i) total simulation time, (ii) geometry of container, (iii) temperature parameters, (iv) evaporation parameters, (v) solver selection and related parameters, (vi) release rate parameters, and (vii) corrosion parameters. The baseline SCCEX code input file is listed in Table B-1.

The output files for this code include the following:

File Name	Data Information			
Sccsml.dat (see Table B-2)	Summarizes the weight factor, the failure time, the time-to-wetting, and the time to leach for all calculation cells in each realization vector.			
mechanical.out (see Table B-3)	Summarizes the temperature, wetted area, remaining thickness of the container, and leachate in each time step. This file will be read by mechanical subroutines to determine failure or not.			
simple.out (see Table B-4)	Data file for plotting purpose.			
main.out (see Table B-5)	Data file for plotting purpose.			
summary.out (See Table B-6)	Summarizes some important results as seen in sccsml.dat.			
release.out (see Table B-7)	Summarizes radionuclide release related information.			

Before running the SCCEX code, there are two steps that must be taken. The first is the removal of any files that may conflict with the SCCEX system output file name. Secondly, the input files must be prepared for the run of interest.

Table B-1. SCCEX Input File

This is the Brine or SCCEX code input file 1000. ! end simulation time 0., 0., 4 !container x,y,z location, number of cells 4.76, 0.33, 0.34, 5.0 ! rlen, r1, r2, r3 0.01 ! container thickness in meters Temperature Parameters 4.44473e8 ! initial power density in J/yr/m² 70000., 2.3, 10.! metric ton initial heavy metal total, MTIHM can, age of fuel 5.68e7, 3.787e7, 3.26e6! J/yr/m/K thermal conductivity for rock, packing, can 2.4e6, 1.2e6, 1.2e6 ! rho*Cp in J/m^3/K, rock, packing, can 23., 4.0 ! initial temperature (Celsius) and vertical extent of repository **Evaporation Parameters** 962., 59., 1.0, 1.0 ! D (m²/yr), tdiff (C), tau rock, tau packing 0.12, 0.12, 2.e-3 ! phi rock, phi pac, water film thick (m) 6 ! ndrip, the number of time, drip rate pairs 0., 1.e-3 ! time in yr, drip rate in m/yr 100., 1.e-3 400., 1.e-3 3000., 1.e-3 8000., 1.e-3 100000., 1.e-3 0.0613, 0.2121 ! salt (Kg/m³), scale (Kg/m³) 1.0 ! bfact, scale factor for vapor pressure lowering relative to NaCl solution 0.1, 0.0 ! initial salt (Kg), initial scale (Kg) 1, 1.0 ! idrip (0 = > no umbrella, 1 = > umbrella effect), gfrac in m² 20., 95, 2. ! slice, tenhan, tslop 0.895 ! atmospheric pressure (atm) 1.e-3, 1.39e-4 ! alt, lambda 1.e-3, 1.e0, 1 ! dt ini, dtmax, isolve 0-> full, 1-> local equilibrium 1.e-3, 1.e-3 ! relative error, absolute error 10., 0.01 !Evap/Qin factor, Vwater/Vcrit factor to switch from local equilibrium **Corrosion Parameters** 0.75, 0.5 ! betaox, betahy 3.e10, 3.2, 100000., 20000. ! rkox, rkhy, Gox, Ghy 6.3e2, 6.3e6 ! curair, curact 6.3e4, 0.0, 0.0 ! aa(1), const., const. 0.0, 0.0, 0.0, 0.0, 0.0, 0.0 ! CEcrit, Counter, const., const., const., const. 1.0, 7.0 ! nitrate/cl ratio, reference pH

0.3, 0.5 ! tortuosity in scale, porosity in scale

Table B-2. Output File — SCCSML.DAT

***** SCCEX FAILURE, WETTING, LEACHATE TIME *****

1 ! total calculation groups

1 ! counter

4 ! weight factor

- 785.00 4 ! failure time, type (0: No failure, 1: Buckling, 2: Fracture, 3: Yield, 4: Corrosion)
- 735.00 1 ! wetting time, type (0: no wet, 1: wet)

1000.00 0 ! leachate time, type (0: no leachate, 1: leachate)

Table B-3. Output File - MECHANICAL.OUT

```
1 4 101 1 ! Counter, weight factor, total time steps, calculation cells
 1 0.100E-02 0.145E+03 0.100E-01 0.000E+00 0.000E+00
 !(time step, years, temperature, remaining thickness, wetted area, leachate)
 2 0.100E+02 0.154E+03 0.100E-01 0.000E+00 0.000E+00
 3 0.200E+02 0.155E+03 0.100E-01 0.000E+00 0.000E+00
 4 0.300E+02 0.152E+03 0.100E-01 0.000E+00 0.000E+00
 5 0.400E+02 0.148E+03 0.100E-01 0.000E+00 0.000E+00
 6 0.500E+02 0.143E+03 0.100E-01 0.000E+00 0.000E+00
 7 0.600E+02 0.139E+03 0.100E-01 0.000E+00 0.000E+00
 8 0.700E+02 0.135E+03 0.100E-01 0.000E+00 0.000E+00
 9 0.800E+02 0.132E+03 0.100E-01 0.000E+00 0.000E+00
10 0.900E+02 0.128E+03 0.100E-01 0.000E+00 0.000E+00
11 0.100E+03 0.126E+03 0.100E-01 0.000E+00 0.000E+00
12 0.110E+03 0.124E+03 0.100E-01 0.000E+00 0.000E+00
13 0.120E+03 0.122E+03 0.100E-01 0.000E+00 0.000E+00
14 0.130E+03 0.120E+03 0.100E-01 0.000E+00 0.000E+00
15 0.140E+03 0.119E+03 0.100E-01 0.000E+00 0.000E+00
16 0.150E+03 0.117E+03 0.100E-01 0.000E+00 0.000E+00
* 17-95 or 160-940 years data
96 0.950E+03 0.927E+02 -0.413E-04 0.676E+01 0.000E+00
97 0.960E+03 0.925E+02 -0.416E-04 0.730E+01 0.000E+00
98 0.970E+03 0.924E+02 -0.418E-04 0.641E+01 0.000E+00
99 0.980E+03 0.922E+02 -0.420E-04 0.659E+01 0.000E+00
100 0.990E+03 0.921E+02 -0.423E-04 0.685E+01 0.000E+00
101 \quad 0.100E + 04 \quad 0.919E + 02 \quad -0.425E - 04 \quad 0.718E + 01 \quad 0.000E + 00
```

). 52

12 -

time, tcan(i), tout(i), tcan(i)-tout(i),

```
vpin, vpout, vpin*.75, erate (m^3/y), e(m^3/m^2/y)
```

! (time, canister surface temp., outer temp., temp. diff., vapor pressure inside, vapor pressure outside, 0.75*vapin, evaporation rate, evaporation rate)

```
0.00E+00 1.45E+02 2.30E+01 1.22E+02 4.23E+00 4.19E-02 3.18E+00 1.00E+00 1.01E-01
1.00E+01 1.54E+02 5.97E+01 9.43E+01 5.33E+00 1.94E-01 4.00E+00 1.00E+00 1.01E-01
2.00E+01 1.55E+02 7.61E+01 7.86E+01 5.41E+00 3.98E-01 4.06E+00 1.00E+00 1.01E-01
3.00E+01 1.52E+02 8.51E+01 6.67E+01 5.06E+00 5.74E-01 3.79E+00 1.00E+00 1.01E-01
4.00E+01 1.48E+02 9.05E+01 5.73E+01 4.54E+00 7.06E-01 3.41E+00 1.00E+00 1.01E-01
5.00E+01 1.43E+02 9.37E+01 4.98E+01 3.99E+00 7.96E-01 2.99E+00 1.00E+00 1.01E-01
6.00E+01 1.39E+02 9.55E+01 4.37E+01 3.44E+00 8.51E-01 2.58E+00 1.00E+00 1.01E-01
7.00E+01 1.35E+02 9.65E+01 3.87E+01 2.94E+00 8.81E-01 2.20E+00 1.00E+00 1.01E-01
8.00E+01 1.32E+02 9.69E+01 3.48E+01 2.48E+00 8.94E-01 1.86E+00 1.00E+00 1.01E-01
9.00E+01 1.28E+02 9.70E+01 3.15E+01 2.22E+00 8.96E-01 1.67E+00 1.00E+00 1.01E-01
1.00E+02 1.26E+02 9.69E+01 2.91E+01 2.15E+00 8.93E-01 1.61E+00 1.00E+00 1.01E-01
1.10E+02 1.24E+02 9.67E+01 2.71E+01 2.08E+00 8.88E-01 1.56E+00 1.00E+00 1.01E-01
1.20E+02 1.22E+02 9.65E+01 2.54E+01 2.02E+00 8.81E-01 1.51E+00 1.00E+00 1.01E-01
1.30E+02 1.20E+02 9.63E+01 2.39E+01 1.96E+00 8.73E-01 1.47E+00 1.00E+00 1.01E-01
1.40E+02 1.19E+02 9.60E+01 2.26E+01 1.88E+00 8.64E-01 1.41E+00 1.00E+00 1.01E-01
1.50E+02 1.17E+02 9.57E+01 2.14E+01 1.80E+00 8.55E-01 1.35E+00 1.00E+00 1.01E-01
```

* 160-940 years data

```
*
```

9.50E+029.27E+018.63E+016.36E+007.65E-016.03E-015.73E-017.17E-017.27E-029.60E+029.25E+018.62E+016.31E+007.60E-016.00E-015.70E-016.97E-017.06E-029.70E+029.24E+018.61E+016.26E+007.56E-015.98E-015.67E-016.77E-016.86E-029.80E+029.22E+018.60E+016.21E+007.52E-015.96E-015.64E-016.58E-016.67E-029.90E+029.21E+018.59E+016.16E+007.48E-015.93E-015.61E-016.40E-016.49E-021.00E+039.19E+018.58E+016.11E+007.44E-015.91E-015.58E-016.21E-016.30E-02

Table B-5. Output File — MAIN.OUT

time, Vwater, KgNaCl, depth, Qout, Kg scale, %NaCl, corr rate, Ecorr, Tcan, Qin !(time, volume of water, Kg of NaCl, corrosion depth, effluent drip rate, Kg of scale, NaCl percent, corrosion rate, Corrosion potential, canister surface temp., drip rate) 1.00E-03 0.00E+00 1.00E-01 2.40E-11 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.45E+02 0.00E+001.00E+01 0.00E+00 1.00E-01 2.40E-07 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.54E+02 0.00E+002.00E+01 0.00E+00 1.00E-01 4.79E-07 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 $1.55E+02 \quad 0.00E+00$ 3.00E+01 0.00E+00 1.00E-01 7.19E-07 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.52E+02 0.00E+004.00E+01 0.00E+00 1.00E-01 9.59E-07 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.48E+02 0.00E+005.00E+01 0.00E+00 1.00E-01 1.20E-06 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.43E+02 0.00E+006.00E+01 0.00E+00 1.00E-01 1.44E-06 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.39E+02 0.00E+007.00E+01 0.00E+00 1.00E-01 1.68E-06 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.35E+02 0.00E+008.00E+01 0.00E+00 1.00E-01 1.92E-06 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.32E+02 0.00E+009.00E+01 0.00E+00 1.00E-01 2.16E-06 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.28E+02 0.00E+001.00E+02 0.00E+00 1.00E-01 2.40E-06 0.00E+00 0.00E+00 2.75E+01 2.40E-08 -9.00E+00 1.26E+02 0.00E+001.10E+02 0.00E+00 3.23E-01 2.64E-06 0.00E+00 7.71E-01 2.75E+01 2.40E-08 -9.00E+00 1.24E+02 4.04E-01 1.20E+02 0.00E+00 5.71E-01 2.88E-06 0.00E+00 1.63E+00 2.75E+01 2.40E-08 -9.00E+00 1.22E+02 4.04E-01 1.30E+02 0.00E+00 8.18E-01 3.12E-06 0.00E+00 2.49E+00 2.75E+01 2.40E-08 -9.00E+00 1.20E+02 4.04E-01 1.40E+02 0.00E+00 1.07E+00 3.36E-06 0.00E+00 3.34E+00 2.75E+01 2.40E-08 -9.00E+00 1.19E + 02 4.04E - 011.50E+02 0.00E+00 1.31E+00 3.59E-06 0.00E+00 4.20E+00 2.75E+01 2.40E-08 -9.00E+00 1.17E+02 4.04E-01 * 160-940 years data 9.50E+02 1.35E-02 4.00E+00 1.00E-02 0.00E+00 1.35E+01 2.28E+01 2.40E-08 -9.00E+00 9.27E+01 1.00E-03 9.60E+02 1.46E-02 4.00E+00 1.00E-02 0.00E+00 1.35E+01 2.15E+01 2.40E-08 -9.00E+00 9.25E+01 1.00E-03 9.70E+02 1.28E-02 4.01E+00 1.00E-02 0.00E+00 1.35E+01 2.38E+01 2.40E-08 -9.00E+00 9.24E+01 1.00E-03 9.80E+02 1.32E-02 4.01E+00 1.00E-02 0.00E+00 1.35E+01 2.33E+01 2.40E-08 -9.00E+00 9.22E+01 1.00E-03 9.90E+02 1.37E-02 4.01E+00 1.00E-02 0.00E+00 1.35E+01 2.26E+01 2.40E-08 -9.00E+00 9.21E+01 1.00E-03 1.00E+03 1.44E-02 4.01E+00 1.00E-02 0.00E+00 1.35E+01 2.18E+01 2.40E-08 -9.00E+00 9.19E+01 1.00E-03

Table B-6. Output File - SUMMARY.OUT

1 101 4 !calculation cell, points/cell, total cells

4 0.571E+03 0.571E+03 0.731E+03 0.963E+02 0.100E+04 0.000E+00 0.790E+03 (Weight factor, x axis position, y axis position, time of first wetting, temp. at first wetting, time of effluent generation, temp. at first effluent, time to fail)

Table B-7. Output File — RELEASE.OUT

time step, fractional radionuclide release /yr, proportion of initial inventory in waste, proportion of initial inventory in waste package water, proportion of initial inventory in waste released from wp, radionuclide output t 2 3 4

1.00E-04 (0.00E + 00	1.00E + 00	0.00E + 00	0.00E+00	0.00E+00		
1.00E+01	0.00E + 00	9.99E-01	0.00E + 00	0.00E + 00	0.00E+00		
2.00E+01	0.00E + 00	9.97E-01	0.00E + 00	0.00E + 00	0.00E+00		
3.00E+01	0.00E+00	9.96E-01	0.00E + 00	0.00E + 00	0.00E+00		
4.00E+01	0.00E + 00	9.94E-01	0.00E + 00	0.00E + 00	0.00E + 00		
5.00E+01	0.00E+00	9.93E-01	0.00E + 00	0.00E + 00	0.00E + 00		
6.00E+01	0.00E+00	9.92E-01	0.00E + 00	0.00E + 00	0.00E + 00		
7.00E+01	0.00E+00	9.90E-01	0.00E + 00	0.00E + 00	0.00E+00		
8.00E+01	0.00E + 00	9.89E-01	0.00E + 00	0.00E + 00	0.00E + 00		
9.00E+01	0.00E+00	9.88E-01	0.00E + 00	0.00E + 00	0.00E + 00		
1.00E+02	0.00E+00	9.86E-01	0.00E + 00	0.00E+00	0.00E+00		
1.10E+02	0.00E + 00	9.85E-01	0.00E + 00	0.00E+00	0.00E + 00		
1.20E+02	0.00E + 00	9.83E-01	0.00E + 00	0.00E+00	0.00E + 00		
1.30E+02	0.00E+00	9.82E-01	0.00E + 00	0.00E+00	0.00E + 00		
1.40E+02	0.00E+00	9.81E-01	0.00E + 00	0.00E+00	0.00E + 00		
1.50E+02	0.00E+00	9.79E-01	0.00E + 00	0.00E+00	0.00E + 00		
*							
* 160-940 years data							
*							
9.50E+02	0.00E + 00	7.36E-01	1.41E-01	0.00E + 00	0.00E + 00		
9.60E+02	0.00E+00	7.26E-01	1.49E-01	0.00E + 00	0.00E+00		
9.70E+02	0.00E+00	7.16E-01	1.58E-01	0.00E + 00	0.00E + 00		
9.80E+02	0.00E+00	7.06E-01	1.66E-01	0.00E + 00	0.00E + 00		
9.90E+02	0.00E + 00	6.97E-01	1.75E-01	0.00E + 00	0.00E + 00		
1.00E+03	0.00E + 00	6.87E-01	1.83E-01	0.00E + 00	0.00E + 00		
APPENDIX C EXAMPLE OF INPUT AND OUTPUT FILES FOR SMLEXC CODE

EXAMPLE OF INPUT AND OUTPUT FILES FOR SMLEXC CODE

As discussed in Section 2, the SMLEXC code contained four basic parts: (i) the executive; (ii) algorithm to sample from statistical distributions; (iii) preprocessor for the SCCEX code input, and (iv) SCCEX code to compute the time-to-failure and the time-to-first-wetting. The input files required are:

File Name	Data Information
smlexc.inp (see Table C-1)	A SMLEXC input file which provides the global run parameters for the executive and the subprocesses. Here the executive control parameters are specified along with the LHS and SCCEXP file names. A start time of 0 years and a stop time of 1,000 years were used for the results in the report. Also, LHS produced 100 sample vectors for the 49 sampled random variables.
smllhs.dat (see Table C-2)	A LHS input file which defines random variables' bounds and distributions.
scpmap.dat (see Table C-3)	This file contains the location information for all of the sampled random variables in the LHS output file.
sccex.inp	This is a standard input file for the standalone version of the SCCEX code (see Table B-1). It is used to present the default values to the SCCEX preprocessor module, when running in system mode. The specification of a hot, warm, or cold run is made by altering the temperature parameters (e.g., initial power density) in the file. Any sampled variables overwrite the default values before the SCCEX input file is generated.

The SMLEXC input file is prepared in a free format style. That is, the input values are associated with keywords rather than fixed column position in the input file. This was implemented using a set of standard FORTRAN routines described in document CNWRA 91-005 (Janetzke and Sagar, 1991).

In addition to these input files, a temporary input file, scpscc.dat (see Table C-4), has been created for transmitting control parameters to the SCCEX code. This temporary file receives its name from the SMLEXC executive and is overwritten for each new vector processed. In general, only the programmer (and not the end user) needs to accommodate the temporary files. This scpscc.dat file is constructed by mapping the sampled data from LHS code to SCCEX code default input file, sccex.inp.

The output files are:

F

File Name	Data Information
lhs.out (see Table C-5)	Summarize sampled data from LHS subprocess.

File Name	Data Information
Fail.cdf and wet.cdf (see Table C-6)	Both files contain the CDF curve for the canister event times indicated in the file name. The event times are collected in an array in the executive after each vector realization and the times are weighted according to the cell weighting factor used by SCCEX.
Postdd.dat	Postdd.dat is used to collect the most valuable information for every system code analysis. More detailed discussions can be seen in Appendix D.
SCCEX code outputs	As discussed in Appendix B.

Before running the SMLEXC system there are two steps that must be taken. The first is the removal of any files that may conflict with the SMLEXC system output file names. Second, the input files must be prepared for the run of interest. The files that should be removed before running the system code are *_TLY*, lhs.out, smlexc.log, smlexc.out, and postdd.dat.

REFERENCE

Janetzke, R.W., and B. Sagar. 1991. RDFREE: A Fortran Utility for Format Free Input. User's Guide. CNWRA 91-005. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.

analyst 'Ron Janetzke' \\ Scenario section.\\ scenario \ Begin first scenario. name 'SCN 01' \ Scenario name. output 'name 1.cum' \ Scenario output file name. ccdf 'sccdf.dat' \ Produce CCDF output. probability 1.0 \ Scenario probability. start time = 0\ Simulation start time. stop time = 1000\ Simulation stop time. 1 lhs \ Specify LHS parameters. vectors = 100\ Number of vectors for this scenario. input '../lhs3/smllhs.dat' \ LHS input file name. output 'lhs.out' \ LHS output file name. SCCEXP input = 'sccex.inp' lhsmap = '../sccexp/scpmap.dat' output = 'scpscc.dat' SCCEX run scenario end \\ Calculation section. \\ output on screen ccdf

TITLE: SMLEXC, 100 vectors, warm, 304L production run II.

END

Table C-1. SMLEXC Input File — SMLEXC.INP

Table C-2. LHS CODE Input File - SMLLHS.DAT

TITLE - LHS input fi	ile for S	CCEX p	arameters. Production run. 9-17-93
RANDOM SEED -	169	*	
NOBS 2			
NREPS 1			
UNIFORM	age	[years]	; Age of fuel.
10.0 60.0			
UNIFORM	tkr	[J/yr/m/	K]; Thermal conductivity for rock.
4.7e7 6.8e7	.1	••• · ·	
$\frac{1}{2} \frac{1}{7} \frac{1}{2} \frac{1}$	tkp	[J/yr/m/	(K); Thermal conductivity for packing.
UNIFORM	rhoenr	[]/m**	3/K1. Density that appaits for real-
2.e6 3.e6	moepi	[J/III	S/K], Density heat_capacity for fock.
LOGUNIFORM	taur	п	· Geometric factor for rock
0.01 1.	tuut	u	, dometric racior for fock.
UNIFORM	phir	Π	: Porosity for rock.
0.05 0.2	•		, ,
UNIFORM	delta	[m]	; Water film thickness.
1.0e-3 3.0e-3			
UNIFORM	salt	[kg/m**	3] ; Salt concentration.
0.05 0.2			.,
UNIFORM	scale	[kg/m**	*3] ; Scale concentration.
0.0 0.5			
UNIFORM	bfact	0	; Vapor pressure lowering scale factor.
0.7 1.3			
UNIFORM	dsalt	[kg]	; Initial salt.
0.0 5.0			
UNIFORM	dscale	[kg]	; Initial scale.
0.0 15.0			
LOGUNIFORM	dfrac	c [m**	[2] ; Funnel area
0.1 10.0			
UNIFORM	slice	[m]	; Umbrella edge thickness.
1.0 30.0			
UNIFORM	tenhan	[C]	; Umbrella edge temperature.
90.0 98.0	. 1		
UNIFORM	tslop	[C]	; +/- range of 'tenhan'.
	1	n	
ONIFORM	Detaox	IJ	; oxygen beta kinetics parameter.
U.2J I.J	h		
0.25 0.5	betany	IJ	; water beta kinetics parameter.
	alson	() * //	
$3 \circ 6 = 3 \circ 14$	rkox	[C*m/(m	ole yr); constant for oxygen reduction.
J.CO J.CI4	rkh	[<u>()</u>	*un)], soto constant for
2 7 <u>0.4</u> 2 704	ikiiy j	[C/(m™m	(yi); rate constant for water reduction.
5.25-7 5.264 CONSTANT	Gov	[]/	1. A attiviation on any for a survey of
100000.	UUX	[1/IIIO	, Activation energy for oxygen rate.

CONSTANT	Ghy	[J/mol]	; activation energy for water rate.
20000.			
UNIFORM	curair	[C/(yr*n	n*m)]; current density for air/steam.
6.3 6.3e3			
UNIFORM	curact	[C/(yr*r	n*m)]; active current density.
6.3e5 6.3e8			
UNIFORM	aa(1)	[C/(yr*n	n*m)] ; cpass coefficient.
6.3e3 6.3e5			
CONSTANT	aa(2)	[]	; cpass coefficient.
0.0			
CONSTANT	aa(3)	0	; cpass coefficient.
0.0			
UNIFORM	CEcrit	0	; Ecrit coefficient.
0. 1.			
CONSTANT	bb(2)	0	; Ecrit coefficient.
0.0			
CONSTANT	bb(3)	0	; Ecrit coefficient.
0.0			
CONSTANT	bb(4)	0	; Ecrit coefficient.
0.0			
CONSTANT	bb(5)	Π	; Ecrit coefficient.
0.0		.,	
CONSTANT	bb(6)	n	: Ecrit coefficient.
0.0	. ,	C)	,
CONSTANT	clrat	ก	: nitrate/chloride ratio.
1.0			· · · · · · · · ·
UNIFORM	taus	n :	tortuosity correction for scale.
0.1 1.0			
UNIFORM	spor	n :	scale porosity.
0.2 1.0	- F		, p, -
CONSTANT	ndrip	[count]	: Number of drip rate values
6.		[•••••••]	, rumou or unp ruto valuos.
CONSTANT	atime()	() [vears]	: Time for adrin
0.	1	-) []•••••0]	, mine for quilp.
CONSTANT	atime(2) [vears]	· Time for adrin
100.	4	J) [Jours]	, mie for quip.
CONSTANT	atime(3) [vears]	· Time for advin
400.	4) [] curo]	, rime for quilp.
CONSTANT	atime(4	1) [vears]	· Time for advin
3000.	denno(i) [Jours]	, Thie for quip.
CONSTANT	atime(4	5) [vears]	· Time for adrin
8000	denuo(:) [Joars]	, This for quip.
CONSTANT	atime(5) [vears]	· Time for adrin
100000	quinc() [years]	, Thie for quilp.
LOGNORMAI	adrin	(1) [m/w	· Infiltration
1 0E-4 5 0E-3	darih	(1) [m/y	, minitation.
LOGNORMAI	adrin	(2) [m/m]	·] · Infiltration
1.0E-4 5.0E-3	dauh	(2) [m/yi	., minication.

LOGNORMAL	qdrip(3) [m/yr]	; Infiltration.
1.0E-4 5.0E-3		
LOGNORMAL	qdrip(4) [m/yr]	; Infiltration.
1.0E-4 5.0E-3		-
LOGNORMAL	qdrip(5) [m/yr]	; Infiltration.
1.0E-4 5.0E-3		·
LOGNORMAL	qdrip(6) [m/yr]	; Infiltration.
1.0E-4 5.0E-3		•

Table C-3. MAPPING Input File - SCPMAP.DAT

```
TITLE: SCCEXP map file for LHS variables.
VERSION: 05-17-93; Original with 6 element qtime & qdrip arrays.
32 variables = 28 scalars + 4 arrays = 49 data values.
VARIABLE INDEX COUNT
'age'
      1
           1
'tkr'
       2
           1
'tkp'
       3
           1
'rhocpr' 4
           1
'taur' 5
            1
'phir' 6
           1
'delta' 7
           1
'salt' 8
           1
'scale' 9
           1
'bfact' 10
           1
'dsalt' 11
            1
'dscale' 12
           1
'dfrac' 13
           1
'slice' 14
            1
'tenhan' 15
           1
'tslop' 16
           1
'betaox' 17
            1
'betahy' 18
            1
'rkox' 19
            1
'rkhy' 20
            1
'Gox'
       21
            1
'Ghy' 22
            1
'curair' 23
            1
'curact' 24
           1
'aa'
      25
           3
'bb'
       28
           6
'clrat' 34
           1
'taus' 35
           1
'spor' 36
           1
'ndrip' 37
            1
'qtime' 38
            6
```

'qdrip' 44

6

Table C-4. SCCEX CODE Input File — SCPSCC.DAT

TITLE: Standard input file for program SCCEX 1000.0 Simulation end time. 0.0 0.0 0.0 256 !Container location x,y,z, number of cells. 4.76 0.33 0.34 5.00 !Cont len, rad, pack rad, outer boundary. 1.00000E-02 !Container thickness in meters. Temperature parameters. 4.44473E+08 !Initial power density in J/yr/m**2. 70000.0 2.30 23.571 !Initial MTHM, MTHM/can, age of fuel. 6.471E+07 4.192E+07 3.260E+06 !Therm cond rock, pack, can. 2.632E+06 1.200E+06 1.200E+06 !Dens*heat cap rock, pack, can. 23.0000 4.00000 !Initial temp(C), vertical extent of repository. Evaporation Parameters. 0.0 0.365 1.00 !Diff,tdiff,geom factor rock, pack. 962.0 1.447E-01 1.200E-01 1.973E-03 !Por rock, pack, water film thick. 6 !Number of drip rate entries. 0.0 7.703E-04 !Time(yr), drip rate(m/yr). 100.0 8.899E-04 !Time(yr), drip rate(m/yr). 400.0 5.556E-04 !Time(yr), drip rate(m/yr). 3000.0 2.841E-04 !Time(yr), drip rate(m/yr). 8000.0 7.360E-04 !Time(yr), drip rate(m/yr). 100000.0 1.352E-03 !Time(yr), drip rate(m/yr). 0.115811 0.142650 !Concentration salt(kg/m**3), scale (kg/m**3). 1.00041 !Scale factor for vapor pressure lowering relative to NaCl sol. 2.09333 9.15491 !Initial salt(kg), scale(kg). 1 6.48606 !idrip=0=> no umbrella, qfrac(m^{**2}). 7.852 93.891 3.152 !slice, tenhan, tslop(+/-tenhan). 0.895000 !Atmospheric pressure (atm). 1.00000E-03 1.39000E-04 !Alteration rate(alt), decay rate (lambda). 1.0E-03 1.0E+00 1 !dt init, dt max, 0 = full, 1 = local equilibrium 1.0E-03 1.0E-03 !relative error, absolute 1.00E+01 1.00E-02 !Evap/Qin, Vwater/Vcrit to switch from local eq. Corrosion Parameters 7.767E-01 4.856E-01 !betaox, betahy 3.592E+12 2.974E+04 1.000E+05 2.000E+04 !rkox, rkhy, Gox, Ghy 2.171E+03 5.314E+08 !curair, curact 4.422E+05 0.000E+00 0.000E+00 !aa(1) ... aa(3) 9.475E-01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 !bb(1) ... bb(6) 1.0E+00 7.0E+00 !nitrate/cl, reference pH 4.416E-01 2.338E-01 !scale tortuosity, porosity

Table C-5. Output File – LHS.OUT

An example lhs.out file which contains one hundred vectors is used to demonstrate the idea. Due to limited space, only the first and last two vectors are shown.

```
1
                 49 ! vector 1, 49 parameters
0.5955357E+02 0.6071842E+08 0.3201504E+08 0.2056904E+07 0.5035967E-01
0.1433044E+00 0.2962184E-02 0.1565893E+00 0.2667075E+00 0.1223796E+01
0.3083017E+01 0.2881417E+01 0.1161487E+01 0.1933476E+02 0.9294939E+02
0.8337170E+00 0.1435763E+01 0.3119096E+00 0.2848598E+15 0.1741379E+05
0.1000000E+06 0.2000000E+05 0.6308075E+03 0.2276032E+09 0.1007032E+06
0.000000E+00 0.000000E+00 0.2558273E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.1000000E+01 0.2868533E+00
0.4607189E+00 0.6000000E+01 0.0000000E+00 0.1000000E+03 0.4000000E+03
0.3000000E+04 0.8000000E+04 0.1000000E+06 0.7228362E-03 0.1275374E-02
0.5719220E-03 0.8524279E-03 0.5524678E-03 0.9388926E-03 ! 49 sampled data
       2
                 49
0.1643093E+02 0.6030909E+08 0.3740568E+08 0.2427813E+07 0.3475545E+00
0.6787387E-01 0.2271059E-02 0.1020446E+00 0.7689659E-01 0.1211360E+01
0.1575169E+01 0.5191948E+01 0.5444325E+01 0.2891110E+02 0.9746048E+02
0.3195549E+01 0.1270932E+01 0.4635397E+00 0.1972573E+15 0.2687916E+05
0.1000000E+06 0.2000000E+05 0.1526452E+03 0.3473426E+09 0.3333916E+05
0.000000E+00 0.000000E+00 0.5412406E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.1000000E+01 0.9306332E+00
0.2932201E+00 0.6000000E+01 0.0000000E+00 0.1000000E+03 0.4000000E+03
0.3000000E+04 0.8000000E+04 0.1000000E+06 0.8861566E-03 0.8796123E-03
0.1722950E-02 0.7543041E-03 0.5164781E-03 0.1544008E-0
       * vectors 3 - 99
       *
      100
                 49
0.2357107E+02 0.6470730E+08 0.4192481E+08 0.2631628E+07 0.3653558E+00
0.1446920E+00 0.1972897E-02 0.1158106E+00 0.1426495E+00 0.1000415E+01
0.2093332E+01 0.9154908E+01 0.6486060E+01 0.7851719E+01 0.9389057E+02
0.3151716E+01 0.7767338E+00 0.4855712E+00 0.3591595E+13 0.2973602E+05
0.1000000E+06 0.2000000E+05 0.2170690E+04 0.5314153E+09 0.4421945E+06
0.000000E+00 0.000000E+00 0.9475294E+00 0.0000000E+00 0.000000E+00
0.0000000E+00 0.0000000E+00 0.0000000E+00 0.1000000E+01 0.4415553E+00
0.2337796E+00 0.6000000E+01 0.0000000E+00 0.1000000E+03 0.4000000E+03
0.3000000E+04 0.8000000E+04 0.1000000E+06 0.7702642E-03 0.8899244E-03
0.5556498E-03 0.2841197E-03 0.7359567E-03 0.1351628E-02
```

Fail.cdf for 304L material

Wet.cdf for 304L material

TITLI	E = "CCDF for SMLEXC, 100 vectors,
warm,	304L production run"
VARI	ABLES = Index, Year, CumProba
ZONI	T = "CDF", F = POINT
1	1.4500E+02 2.5000E-03
2	1.5500E+02 2.6562E-03
3	1.8500E+02 4.8437E-03
4	1.9500E+02 5.0000E-03
5	2.0500E+02 7.5000E-03
6	2.3500E+02 7.8125E-03
7	2.4500E+02 1.0781E-02
8	2.5500E+02 1.1250E-02
9	2.6500E+02 1.3437E-02
10	2.7500E+02 1.5312E-02
11	2.8500E+02 1.6094E-02
12	2.9500E+02 1.8750E-02
13	3.0500E+02 2.0312E-02
14	3.1500E+02 2.3125E-02
15	3.2500E+02 2.7031E-02
16	3.3500E+02 3.6406E-02
17	3.4500E+02 4.0781E-02
18	3.5500E+02 4.7656E-02
19	3.6500E+02 4.9219E-02
20	3.7500E+02 5.1250E-02
21	3.8500E+02 5.3750E-02
22	3.9500E+02 5.6406E-02
23	4.0500E+02 6.0156E-02
24	4.1500E+02 6.5000E-02
25	4.2500E+02 6.7812E-02
26	4.3500E+02 6.8125E-02
27	4.4500E+02 6.8437E-02
28	4.5500E+02 6.8594E-02
29	4.6500E+02 6.9375E-02
30	4.7500E+02 7.0469E-02
31	4.8500E+02 7.1719E-02
32	4.9500E+02 7.2500E-02
33	5.0500E+02 7.6406E-02
34	5.1500E+02 7.7187E-02
35	5.2500E+02 8.4687E-02
36	5.3500E+02 8.8125E-02
37	5.4500E+02 9.2031E-02
38	5.5500E+02 9.6094E-02
39	5.6500E+02 9.8906E-02

TITL	E = "CCDF for	SMLEXC,	100
vectors	s, warm, 304L	production ru	n"
VARI	ABLES = Index	,Year,CumPr	oba
ZON	E T="CDF",F	=POINT	
1	1.3500E+02	3.1250E-04	
2	1.4500E + 02	2.5000E-03	
3	1.5500E+02	2.6562E-03	
4	1.8500E+02	1.2500E-02	
5	1.9500E+02	1.2656E-02	
6	2.0500E + 02	1.7031E-02	
7	2.1500E+02	1.7812E-02	
8	2.2500E+02	1.7969E-02	
9	2.3500E+02	2.0469E-02	
10	2.4500E + 02	2.2812E-02	
11	2.5500E+02	2.3281E-02	
12	2.6500E + 02	2.3437E-02	
13	2.7500E+02	2.9375E-02	
14	2.8500E + 02	3.1719E-02	
15	2.9500E+02	3.1875E-02	
16	3.0500E+02	3.4219E-02	
17	3.1500E+02	3.9531E-02	
18	3.2500E+02	4.1875E-02	
19	3.3500E+02	5.1250E-02	
20	3.4500E+02	5.3281E-02	
21	3.5500E+02	5.7656E-02	
22	3.6500E+02	6.4375E-02	
23	3.7500E+02	6.6250E-02	
24	3.8500E+02	6.9062E-02	
25	3.9500E+02	7.5000E-02	
26	4.0500E+02	7.7500E-02	
27	4.1500E+02	8.1406E-02	
28	4.2500E+02	8.5781E-02	
29	4.3500E+02	8.6094E-02	
30	4.4500E+02	8.6406E-02	
31	4.5500E+02	8.6562E-02	
32	4.6500E+02	8.7187E-02	
33	4.7500E+02	8.9219E-02	
34	4.8500E+02	9.0156E-02	
35	4.9500E+02	9.0625E-02	
36	5.0500E+02	9.4375E-02	
37	5.1500E+02	9.5625E-02	
38	5.2500E+02	1.0469E-01	
39	5.3500E+02	1.1000E-01	

40	5.7500E+02	1.0297E-01
41	5.8500E+02	1.0422E-01
42	5.9500E+02	1.1203E-01
43	6.0500E+02	1.1359E-01
44	6.1500E+02	1.1578E-01
45	6.2500E+02	1.2047E-01
46	6.3500E+02	1.2266E-01
47	6.4500E+02	1.2359E-01
48	6.5500E+02	1.2578E-01
49	6.6500E+02	1.2922E-01
50	6.7500E+02	1.3531E-01
51	6.8500E+02	1.4172E-01
52	6.9500E+02	1.4250E-01
53	7.0500E+02	1.4328E-01
54	7.1500E+02	1.4891E-01
55	7.2500E+02	1.5297E-01
56	7.3500E+02	1.5406E-01
57	7.4500E+02	1.5984E-01
58	7.5500E+02	1.6250E-01
59	7.6500E+02	1.6312E-01
60	7.7500E+02	1.6625E-01
61	7.8500E+02	1.6734E-01
62	7.9500E+02	1.6844E-01
63	8.0500E+02	1.7141E-01
64	8.1500E+02	1.7406E-01
65	8.2500E+02	1.7672E-01
66	8.3500E+02	1.7922E-01
67	8.4500E+02	1.7953E-01
68	8.5500E+02	1.8172E-01
69	8.6500E+02	1.8578E-01
70	8.7500E+02	1.8797E-01
71	8.8500E+02	1.8922E-01
72	8.9500E+02	1.9156E-01
73	9.0500E+02	1.9422E-01
74	9.1500E+02	1.9578E-01
75	9.2500E+02	1.9734E-01
76	9.3500E+02	2.0172E-01
77	9.4500E+02	2.0562E-01
78	9.5500E+02	2.0937E-01
79	9.6500E+02	2.1312E-01
80	9.7500E+02	2.1734E-01
81	9.8500E+02	2.1969E-01
82	9.9500E+02	2.2406E-01
83	1.0000E+03	9.9988E-01

40	5.4500E+02	1.1344E-01
41	5.5500E+02	1.1844E-01
42	5.6500E+02	1.1969E-01
43	5.7500E+02	1.2500E-01
44	5.8500E+02	1.2516E-01
45	5.9500E+02	1.3172E-01
46	6.0500E+02	1.3500E-01
47	6.1500E+02	1.3687E-01
48	6.2500E+02	1.3969E-01
49	6.3500E+02	1.4109E-01
50	6.4500E+02	1.4203E-01
51	6.5500E+02	1.4969E-01
52	6.6500E+02	1.5687E-01
53	6.7500E+02	1.6531E-01
54	6.8500E+02	1.7109E-01
55	6.9500E+02	1.7422E-01
56	7.0500E+02	1.7719E-01
57	7.1500E+02	1.8406E-01
58	7.2500E+02	1.8656E-01
59	7.3500E+02	1.8812E-01
60	7.4500E+02	1.9375E-01
61	7.5500E + 02	1.9469E-01
62	7.6500E+02	1.9562E-01
63	7.7500E+02	1.9937E-01
64	7.8500E+02	2.0344E-01
65	7.9500E+02	2.0875E-01
66	8.0500E+02	2.1500E-01
67	8.1500E+02	2.1656E-01
68	8.2500E + 02	2.2094E-01
69	8.3500E+02	2.2312E-01
70	8.4500E+02	2.2578E-01
71	8.5500E+02	2.2969E-01
72	8.6500E+02	2.3344E-01
73	8.7500E+02	2.3750E-01
74	8.8500E+02	2.4625E-01
75	8.9500E+02	2.4937E-01
76	9.0500E+02	2.5312E-01
77	9.1500E+02	2.5750E-01
78	9.2500E+02	2.6203E-01
79	9.3500E+02	2.6781E-01
80	9.4500E+02	2.7156E-01
81	9.5500E+02	2.7406E-01
82 01	9.6500E+02	2.7594E-01
٥ <u>٥</u>	9.7500E+02	2.8141E-01
04 0 <i>5</i>	9.8500E+02	2.8687E-01
82 86	9.9500E+02	2.9562E-01
80	1.0000E + 03	9.9992E-01

APPENDIX D OUTPUT DATA FILE – POSTDD.DAT

OUTPUT DATA FILE - POSTDD.DAT

Postdd.dat is used to collect the most valuable information for every system code analysis. This information includes the weight factor, the time-to-failure, the time-to-wetting, and the time-to-leachate for every calculation cell in every simulation vector. These valuable data will then be analyzed by using a postprocessing code called POST to produce data for probabilistic assessment.

A demonstration example which has two simulation vectors and three calculation groups (or total no. of cells = 16) is listed as follows:

***** SCCEX FAILURE, WETTING, LEACHATE TIME ***** ! vector 1 results 3! three calculation groups 1 ! counter 4 ! weight factor (similar cells) 1000, 0 ! failure time, type (0: No failure, 1: Buckling, 2: Fracture, 3: Yield, 4: Corrosion) 1000, 0 ! wetting time, type (0: no wet, 1: wet) 1000, 0 ! leachate time, type (0: no leachate, 1: leachate) 2 8 975, 4 925, 1 1000, 0 3 4 950, 4 900, 1 1000.0 ***** SCCEX FAILURE, WETTING, LEACHATE TIME ***** ! vector 2 results 3 1 4 990, 0 935.0 1000, 0 2 8 955, 4 905.1 1000, 0 3 4 915, 4 875, 1 1000, 0

A Postprocessing Code: POST

POST code is developed mainly to postprocess the system analysis data file, postdd.dat. This code is designed to fully utilize this valuable information by constructing different cumulative distribution functions (CDFs) and probability density functions (PDFs) at user selected total number of cell failures or times to failure. These CDFs and PDFs can easily be used to compare the impact of different material and environmental parameters, to access the potential risk of the system at selected years, and to determine the necessary changes in design materials at selected reliability or probability of failure goals.

POST code is an interactive code which is very convenient for the user to use, however, the user must understand how to input the data correctly. To illustrate the idea, a demonstration example for using this program is listed as follows:

post.e ! to start the POST code

```
*** PROBABILISTIC OUTPUT POSTPROCESSOR *** ! title
*** ENTER TOTAL NO. OF VECTORS USED =
100 ! important data in postdd.dat
*** ENTER TOTAL NO. OF GROUPS USED =
36 ! important data in postdd.dat
*** ENTER TOTAL NO. OF CELLS USED =
256 ! important data in postdd.dat
*** ENTER TOTAL SIMULATION TIME USED =
1000 ! important data in postdd.dat
*** ENTER TOTAL NO. OF GROUPS (ACTIVE CELLS) IN EACH VECTOR =
36 ! important data in postdd.dat
*** PROBABILISTIC DISTRIBUTION FOR THE WORST GROUPS ! based on mean value
*** SELECT TOTAL NO. OF GROUPS TO BE CONSTRUCTED =
1
ENTER THE WORST GROUP NO. FOR DISTRIBUTION 1
1
*** PROB. DIST. AT USER-SELECTED TOTAL NO. OF CELL FAILURES
*** SELECT TOTAL NO. OF DISTRIBUTIONS TO BE CONSTRUCTED =
3
ENTER TOTAL NO. OF CELL FAILURES FOR DISTRIBUTION 1
1
ENTER TOTAL NO. OF CELL FAILURES FOR DISTRIBUTION 2
64
ENTER TOTAL NO. OF CELL FAILURES FOR DISTRIBUTION 3
256
```

```
*** PROBABILISTIC DISTRIBUTION AT USER-SELECTED YEARS

*** SELECT TOTAL NO. OF DISTRIBUTIONS TO BE CONSTRUCTED =

3

ENTER SELECTED YEAR FOR DISTRIBUTION 1

300

ENTER SELECTED YEAR FOR DISTRIBUTION 2

650

ENTER SELECTED YEAR FOR DISTRIBUTION 3

1000

*** ENTER DATA INPUT FILE NAME

304lcl.dat ! can be any other names.
```

A total of four data files will be created with this run. The names of these files and their functions are:

Name	Function
"filename".out (304lcl.out)	Data input echo.
"filename".ou1 (304lcl.ou1)	Data used for creating the cdf plots for the worst groups.
"filename".ou2 (304lcl.ou2)	Data used for creating the cdf plots for different total number of cell failures.
"filename"ou3 (304lcl.ou3)	Data used for creating the pdf plots at user selected years.

Based on data stored in 304lcl.ou1, 304lcl.ou2, and 304lcl.ou3, three plots, as shown in Figures 5-1, 5-2, and 5-3, are created.