SCCEX: A COMPUTER CODE FOR SUBSTANTIALLY COMPLETE CONTAINMENT EXAMPLE ANALYSIS OF A REFERENCE CONTAINER VERSION 1.01

Prepared for

Nuclear Regulatory Commission
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Prepared by

Center for Nuclear Waste Regulatory Analyses
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ABSTRACT

The Substantially Complete Containment EXample (SCCEX) computer code is designed to demonstrate an approach for evaluating containment by a waste package and to identify those areas that require more detailed analysis. Several models were coupled in the SCCEX code to calculate the time-to-wetting and the time-to-failure of waste packages for an unsaturated repository site. These models represent the repository thermal field, near-field environment, release rate, corrosion of container materials, including localized corrosion and stress corrosion cracking, and mechanical failures. This user manual discusses the models used in the SCCEX code, code structure and capabilities, input and output files, baseline case, and configuration control status. This code was used to develop an example problem for evaluating the "Substantially Complete Containment" aspects of the Code of Federal Regulations, Title 10, Part 60 (10 CFR Part 60). This version (1.01) differs only slightly from Version 1.0.

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ACKNOWLEDGMENTS

Development of the Substantially Complete Containment EXample (SCCEX) code is a joint effort between the Center for Nuclear Waste Regulatory Analyses (CNWRA), and the Nuclear Regulatory Commission (NRC), Office of Nuclear Material Safety and Safeguards (NMSS), Division of Waste Management (DWM). The authors wish to acknowledge the help of Narasi Sridhar, Prasad K. Nair, and Pavitra Ramanujam in providing technical support and performing some of the computer simulations.

The authors wish to thank Amitava Ghosh, Robert L. Marshall, and Gustavo A. Cragnolino for providing technical reviews and Budhi Sagar and Wesley C. Patrick for their programmatic reviews. The assistance of Lori Salas [Southwest Research Institute (SwRI)], Bonnie L. Garcia (CNWRA), and the SwRI publications staff in producing this document are also acknowledged.

This report was prepared to document work performed by the CNWRA for the NRC under Contract No. NRC-02-93-005. The activities reported were performed on behalf of the NRC NMSS, DWM. The report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC.

QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

The SCCEX code was developed at the CNWRA for the limited purpose of solving an example problem. This code is not expected to become a part of NRC's compliance determination method. However, the code's configuration will be controlled under CNWRA's Technical Operating Procedure 018.

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.

1 INTRODUCTION

The objective of the Substantially Complete Containment EXample (SCCEX) code is primarily to demonstrate an approach for evaluating containment by a waste package and to identify those areas requiring more detailed analysis. SCCEX is not intended to demonstrate the suitability of any given waste package material or design in terms of performance requirements. For simplicity, the failure of a waste package in this analysis is defined as the condition of a waste package in which localized corrosion has penetrated the container walls, either by localized corrosion or by mechanically dominated processes. This computer code can be used in evaluating containment times and other performance factors for waste packages. However, at this stage of development, the model should only be viewed as a research tool and not capable of giving definitive answers.

The code is developed to simulate the performance of the reference waste package design presented in the Site Characterization Plan (SCP) (U.S. Department of Energy, 1988). 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 code. The container materials conform generally to the austenitic alloys described in the SCP. However, the code allows significant departures in the assumptions regarding the chemical and loading environments from those described in the SCP.

The modeling of the near-field environment used in the code is focused on the time-dependent evolution of the chemical environment on the waste package surface. This focus 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, to deposit salts on the waste package surface. This concentration of salts in the presence of future groundwater intrusion can promote and accelerate the corrosion of certain waste package materials. Due to the simplified nature of the models on which the code is based and the assumptions and approximations made, the code does not necessarily provide a quantitative representation of the actual conditions that may be presented in an unsaturated repository site.

Brief overviews of the repository thermal field, near-field environment, release rate, corrosion mechanisms of container materials, including localized corrosion and stress corrosion cracking, as well as mechanical failures models embodied in the SCCEX Version 1.0 software are provided in Section 2. Section 3 contains a general description of the SCCEX software. The required input parameters for the SCCEX code are discussed in Section 4, and the corresponding output files are discussed in Section 5.

2 BRIEF DESCRIPTION OF MODELS

2.1 OVERVIEW

The SCCEX code, developed to assess the 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. In the following subsections, a brief description of these models, which include the repository thermal field, near-field environment, release rate, corrosion of container materials, including localized corrosion and stress corrosion cracking, as well as mechanical failure models is provided. 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) and the report entitled *"Substantially Complete Containment"—Example Analysis of a Reference Container* (Cragnolino et al., 1994). This section is essentially a summary of the description presented in the latter report (Cragnolino et al., 1994).

2.2 THERMAL MODEL

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

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

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

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

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

where

ρC_p = volumetric heat capacity $(Jm^{-3}\,{}^{\circ}K^{-1})$

w = width of square repository (m)

h = height of repository (m)

x,y,z = distance from center of repository (assumed zero) (m)

α = $\kappa/\rho C_p$ = thermal diffusivity (m^2/s)

κ = thermal conductivity $(Wm^{-1}\,°K^{-1})$

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

$$T(x,y,z,t) = \left[\int_0^t Q(\tau) m G(t-\tau)\,d\tau\right] + T_{ref} \qquad (2\text{-}3)$$

where

t = time (s)

Q = heat generation rate per kg of initial heavy metal $(Js^{-1}\,°kg^{-1})$

m = mass of heavy metal (kg)

T_{ref} = initial temperature (23 °C)

The rate of heat generation, Q, is based on data reported by the U.S. Department of Energy (1993). 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 calculated using a steady-state, heat-conduction model for a radial geometry. The quasi-steady-state assumption for variation of the temperature 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 quasi-steady-state temperature difference between the surface of a container and the rock some distance away is given by

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

where

r_1, r_2, r_3 = radial distances of container wall, packing/rock interface, and outer boundary respectively from container centerline (m)

κ_p, κ_r = thermal conductivity of packing and rock, respectively $(Wm^{-1}\,°K^{-1})$

l = length of container (m)

The output of this model is the temperature distribution in Cartesian coordinates 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. A significant limitation of the expression for the temperature drop, ΔT, is that it increases without bound as the radius parameter, r_3, of the outer boundary increases as follows directly from Eq. (2-4). This is a consequcnce of the assumption of a steady state temperature profile and the boundary condition of a fixed temperature at r_3. Unrealistic results may be obtained if the value used for r_3 becomes too large. There is no check of this in the code and the user must evaluate the results to make certain the results are reasonable. Furthermore, the results are generally sensitive to the value of r_3 chosen.

2.3 ENVIRONMENTAL MODEL

In the environmental model, the evolution of the environment on the waste container surface is computed. The environment around the container is dictated by the evaporation rate of water contacting the container, the influx rate of water, the types of salts precipitated, and their effects in reducing the vapor pressure of water on the container surface, which promotes movement of water vapor toward or away from the container surface. The results 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 has a limited thickness. 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.

Several factors are calculated by solving a set of ordinary differential equations representing conservation of mass. These factors include 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. The material balance equations are given by

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

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

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

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

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

where

A_w = fraction of container surface covered with water

V = volume of water on waste container surface (m^3)

Q_{in}, Q_{out} = volumetric flow rate of water onto and exiting the waste container surface (m^3/s)

E = molar evaporation rate from the entire container surface without end effects

M_{H_2O} = molecular weight of water $(kg/kg\ mol)$

ρ_{H_2O} = density of water (kg/m^3)

S = mass of soluble salts on container surface (kg)

s = mass of scale-forming compounds on container surface (kg)

C_{in}, C_{out} = input and output aqueous concentration of soluble salts or scale-forming compounds (kg/m^3)

Γ = cumulative amount of effluent water (m^3)

L = depth of penetration by corrosion (m)

r = corrosion rate, either passive or active (m/s)

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

Liquid water can reach the container surface by several mechanisms including matrix flow, fracture flow, or condensate dripping. Water flow 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 multiplied by the representative area of the individual waste package multiplied by an input factor specifying the proportion of water passing a waste package that actually drips onto the container surface and the evaporation rate.

The second option is more complex and assumes a scenario affecting a larger geometrical area. The imagined scenario is the drying of the repository by the thermal loading. The concept invokes an assumed 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 from the center of the repository to the outer edges, which have temperatures below the boiling point of water. Further 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 specified range. The physical thickness of the umbrella edge (where enhanced flow occurs) and the surface area of impingement are also inputs to the code.

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).

$$N_{H_2O} = x_{H_2O}\left(N_{H_2O} + N_{air}\right) - cD\tau\phi\nabla x_{H_2O} \tag{2-10}$$

where

N_{H_2O} = molar flux of water vapor $(kg\ mol\ m^{-2}s^{-1})$

N_{air} = molar flux of air $(kg\ mol\ m^{-2}s^{-1})$

x_{H_2O} = mole fraction of water vapor

c = total molar concentration of gas $(kg\ mol/m^3)$

D = binary diffusion coefficient (m^2/s)

τ = tortuosity factor

ϕ = rock porosity

Steady-state evaporation in a radial geometry gives

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

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 diffusion coefficient in the air/water vapor system in m^2/s is assumed to be that given by Treybal (1980).

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

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 among vapor pressure, concentration, and mole fraction are performed with the ideal gas law.

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 possibilities 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, $b_{capillary}$, is described with Kelvin's equation.

$$b_{capillary} = \frac{p_{capillary}}{p^0} = \exp\left[\frac{\psi M_{H_2O} g}{RT} \right] \tag{2-13}$$

where

$p_{capillary}$ = vapor pressure of capillary (atm)

p^0 = vapor pressure at temperature for pure water (atm)

ψ = matrix potential (m)

g = acceleration of gravity (m/s^2)

R = gas constant $(J°K^{-1}\ mol^{-1})$

T = temperature $(°K)$

Vapor pressure lowering from solutes, b_{solute}, is a function of concentration and solute composition according to

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

where f represents an arbitrary function of the solution composition specified by concentration C_i of the i^{th} species. Total vapor pressure lowering is a combination of solute and capillary effects given by the equation

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

In the code, the salt that is precipitated is assumed to be sodium chloride. Based on this assumption, the time-to-wetting is calculated 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.

2.4 RELEASE RATE MODEL

Release rate is simulated for a single, highly soluble, radionuclide such as iodine or technetium. Three time periods are identified. Prior to container failure, the spent fuel remains intact, and the radioactive decay is the only active process. Container failure cannot occur until the surface of the container is wetted. The rate of change for each variable before container failure is

$$\frac{d\gamma_1}{dt} = -\lambda\gamma_1$$

$$\frac{d\gamma_2}{dt} = 0 \tag{2-16}$$

$$\frac{d\gamma_3}{dt} = 0$$

After the waste container fails, spent fuel alteration begins. Assuming a zeroth-order rate law for spent fuel alteration, the governing equations during this alteration period are

$$\frac{d\gamma_1}{dt} = -\lambda\gamma_1 - \text{alt} \exp[-\lambda t]$$

$$\frac{d\gamma_2}{dt} = \text{alt} \exp[-\lambda t] - Q_{out}\frac{\gamma_2}{V} - \lambda\gamma_2 \qquad (2\text{-}17)$$

$$\frac{d\gamma_3}{dt} = Q_{out}\frac{\gamma_2}{V}$$

Beyond the alteration period, the governing equations are

$$\frac{d\gamma_1}{dt} = 0$$

$$\frac{d\gamma_2}{dt} = -Q_{out}\frac{\gamma_2}{V} - \lambda\gamma_2 \qquad (2\text{-}18)$$

$$\frac{d\gamma_3}{dt} = Q_{out}\frac{\gamma_2}{V}$$

where

γ_1	=	proportion of initial radionuclide inventory remaining in the unaltered spent fuel
γ_2	=	proportion of initial radionuclide inventory dissolved in the water inside the failed waste package
γ_3	=	proportion of initial radionuclide inventory released from waste package
λ	=	radionuclide decay rate (yr^{-1})
alt	=	alteration rate of spent fuel into secondary minerals (yr^{-1})

The period of alteration extends from the failure time (tfail) to (tfail) + 1/alt. The assumption is made that, prior to the time of leachate generation from the waste package, liquid water flow is always toward the waste package, effectively preventing diffusional and advective releases in the liquid phase (Pruess and Tsang, 1993). Final release from the waste package is assumed to be advectively controlled.

2.5 CORROSION MODEL

The corrosion model in the SCCEX code calculates 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.

2.5.1 Corrosion Potential

Two cathodic reactions are modeled in the code: (i) oxygen reduction, and (ii) 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

$$i_{O_2} = -k_{O_2} C_{O_2}^{bulk} \frac{\exp\left(-\frac{z_{O_2}\beta F E_{corr}}{RT}\right)}{\left[1 + \frac{k_{O_2}\delta \exp\left(-\frac{z_{O_2}\beta F E_{corr}}{RT}\right)}{4FD_{O_2}\tau\phi}\right]} \qquad (2\text{-}19)$$

where

k_{O_2}	=	reaction rate constant for the oxygen reduction reaction ($C \cdot m\ mole^{-1}\ yr^{-1}$)
E_{corr}	=	corrosion potential (mV)
F	=	Faraday constant (Coul/equivalent)
α	=	charge transfer coefficient
β	=	$1 - \alpha$
R	=	gas constant ($kJ\ mol^{-1}\ °K^{-1}$)
T	=	temperature ($°K$)
z_{O_2}	=	number of electrons involved in the process per mole
D_{O_2}	=	diffusivity of oxygen in aqueous solution (m^2/s)
τ	=	tortuosity
ϕ	=	porosity
δ	=	thickness of the diffusion layer (e.g., scale or water film) (m)
$C_{O_2}^{bulk}$	=	bulk concentration of oxygen in solution ($mole/m^3$)

For the oxygen reduction reaction, the bulk concentration is related to the partial pressure through Henry's law

$$C_{O_2}^{bulk} = K_H \cdot p_{O_2} \qquad (2\text{-}20)$$

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 corrosion potential, E_{corr}, 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.

The reaction rate constant is calculated from the exchange current density using the following equation

$$i_{O_2}^0 = k_{O_2} C_{O_2}^{bulk} \exp\left(-\frac{z_{O_2}(1-\alpha)F}{RT} E_{eq}^{O_2}\right) \qquad (2\text{-}21)$$

where

$i_{O_2}^0$ = exchange current density ($amp\ m^{-2}$)

$E_{eq}^{O_2}$ = equilibrium potential for the oxygen evolution reaction (mV)

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

$$i_{H_2O} = -k_{H_2O} \exp\left(-\frac{\beta_{H_2O} z_{H_2O} F}{RT} E_{corr}\right) \qquad (2\text{-}22)$$

where

k_{H_2O} = reaction rate constant for the water reduction reaction ($amp\ m^{-2}$)

E_{corr} = corrosion potential (mV)

The reaction rate constant can be calculated from the appropriate exchange current density for the hydrogen evolution reaction similar to that shown in Eq. (2-21). 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. (2-23).

$$k = k_{298\,^\circ K} \exp\left[\frac{E_a}{R}\left(\frac{1}{298} - \frac{1}{T}\right)\right] \qquad (2\text{-}23)$$

where E_a is the activation energy for the particular cathodic reaction and $k_{298\,^\circ K}$ is the reaction rate constant at 298 °K. The anodic current is assumed to be equal to the passive current density of the alloy and to be independent of the potential. The corrosion potential is then calculated by solving simultaneously for E_{corr} using Eqs. (2-19) and (2-22) and the equality of anodic and cathodic current.

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

Empirically derived equations are used in the SCCEX 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. However, in the present calculations, the effects of these anionic species are not considered. The dependence of the critical potentials on chloride concentration and temperature is given by

$$E_{crit} = A(T) + B(T) \log [Cl^-] \tag{2-24}$$

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

The corrosion potential E_{corr} is calculated by summing the currents to zero. The corrosion rate, r, in Eq. (2-9) is calculated for $E_{crit} < E_{corr}$ according to the expression

$$nFr = i_{act} \qquad (E_{crit} < E_{corr}) \tag{2-25a}$$

and for $E_{crit} > E_{corr}$ by the equation

$$nFr = i_{pass} \qquad (E_{crit} > E_{corr}) \tag{2-25b}$$

where n is the number of electrons taking part in the corrosion reaction. The active i_{act} and passive i_{pass} currents are read in from the input file.

The existence of a critical potential for stress corrosion cracking is less certain; however, it was assumed to be 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 by Sridhar et al. (1993).

2.6 MECHANICAL MODEL

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. Further, it was assumed that there were no momentum losses in the impact and the bottom of the container moved on a frictionless surface. In the calculations involving seismic load, the region of contact with the borehole is assumed to be 10 percent of the circumference of the container. This assumption is conservative, 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 current SCCEX code, an acceleration of 0.4 g seismic load was used. This value is arbitrarily chosen and may not be conservative.

2.6.1 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. The analytical equation used for this buckling failure model is expressed as

$$R_B = \frac{99Et_R^3\pi}{60r^2(1-\nu^2)} \tag{2-26}$$

where

R_B = residual buckling load capacity for the container ($MPa \cdot m$)
E = Young's modulus (MPa)
ν = Poisson's ratio
r = inner radius of the container (m)
t_R = remaining thickness at any given time after accounting for corrosion of the container (m)

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 safety factor equal to two was used for this failure model to add conservatism.

2.6.2 Yield Failure Model

The residual yield capacity, R_Y , was determined (Sridhar et al., 1993) from the following equation

$$R_Y = R_{YO}\frac{A_R}{A} = R_{YO}\frac{t_R}{t} \tag{2-27}$$

where

R_{YO} = yield strength of the material (MPa)
A = initial cross section area of the solid part of the cylinder (m^2)
A_R = remaining cross section area of the solid part of the cylinder (m^2)
t = initial thickness of the cylinder (m)
t_R = remaining thickness of the cylinder after corrosion (m)

A safety factor of two was also incorporated into Eq. (2-26) to provide conservative calculations.

2.6.3 Fracture Failure Model

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

$$R_F = \frac{K_{IC}}{Y(\pi a)^{0.5}} \tag{2-28}$$

where

R_F = permissible external stress (MPa)
Y = geometry factor
a = crack depth or the depth of a corroded pit (m)
K_{IC} = fracture toughness ($MPa\ m^{1/2}$)

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

2.6.4 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 (Cragnolino et al., 1994). It should be noted that the wall thickness is reduced as a result of general or localized 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.

3 SOFTWARE DESCRIPTION

3.1 SCCEX CODE CAPABILITIES

In general, the SCCEX code involves the following calculations:

(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 comparing with predicted evaporation rates.

(iii) Solve a system of ordinary differential equations for
- Volume of water on container surface (m^3)
- 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 for a single radionuclide. The radionuclide is assumed to be highly soluble. Three differential equations are solved: (a) proportion of the initial inventory of the radionuclide remaining in the waste, (b) proportion of the initial inventory in solution in the water that is inside the waste package, and (c) proportion of the initial inventory released from the waste package.

(v) Determine whether or not mechanical failure occurs.

3.2 SCCEX CODE STRUCTURE

The current SCCEX code flow diagram is presented in Figure 3-1. Note that in this version of the code, there is no coupling between the release rate and mechanical modules. The input data required to execute the SCCEX code include the following: (i) total simulation time, (ii) geometry of container, (iii) temperature parameters, (iv) evaporation parameters, (v) release rate and solver parameters, and (vi) corrosion parameters. The input and output structure for the SCCEX code is discussed in detail in the following subsections. 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 3-2. In the SCCEX code, the calculation cells on the diagonal occur four times in the repository, whereas off-diagonal cells occur eight times. The number of times each cell occurs in the repository is called the weighting factor, which is used to calculate the total number of failures in the repository.

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

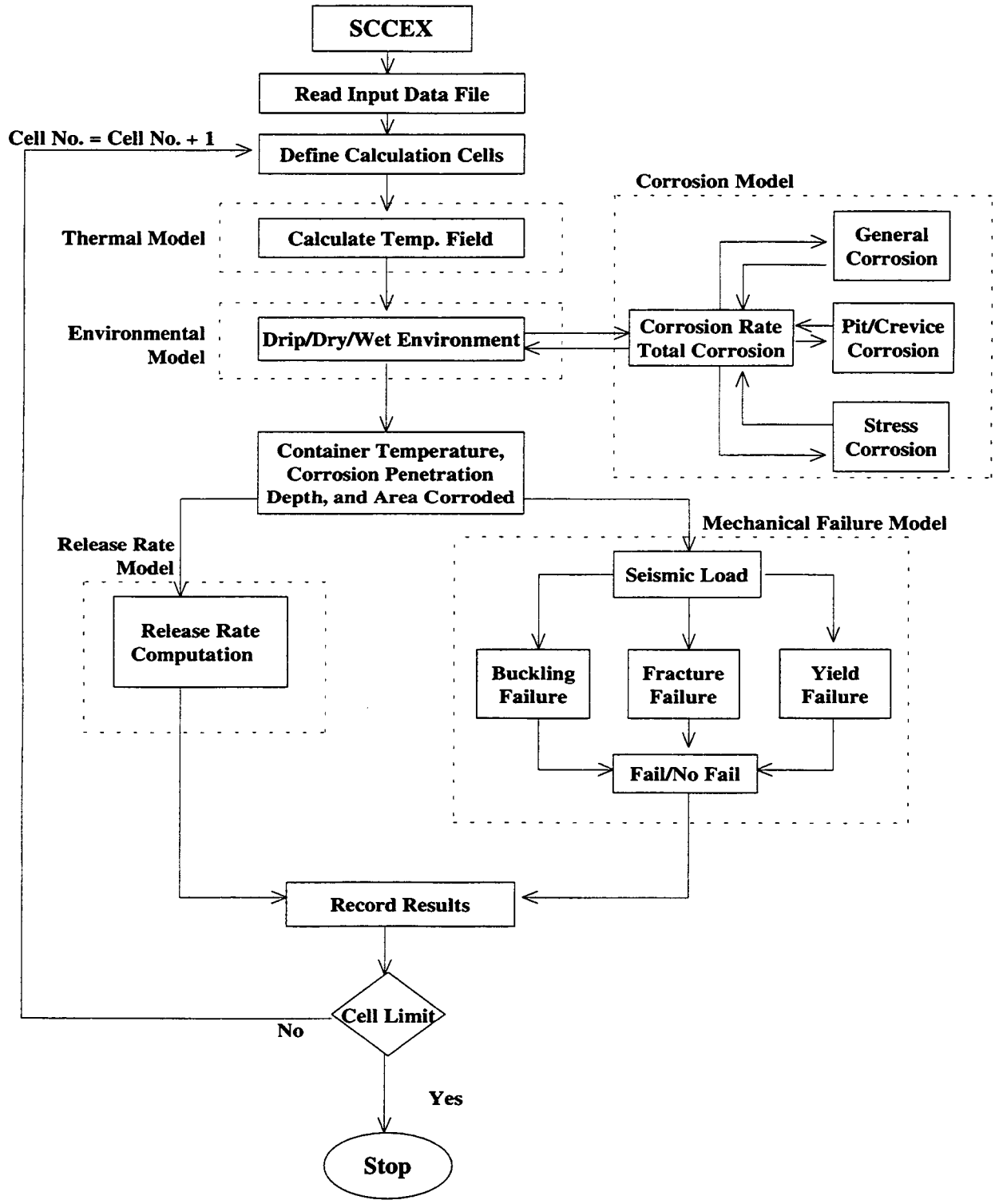

Figure 3-1. Flow diagram of the SCCEX code

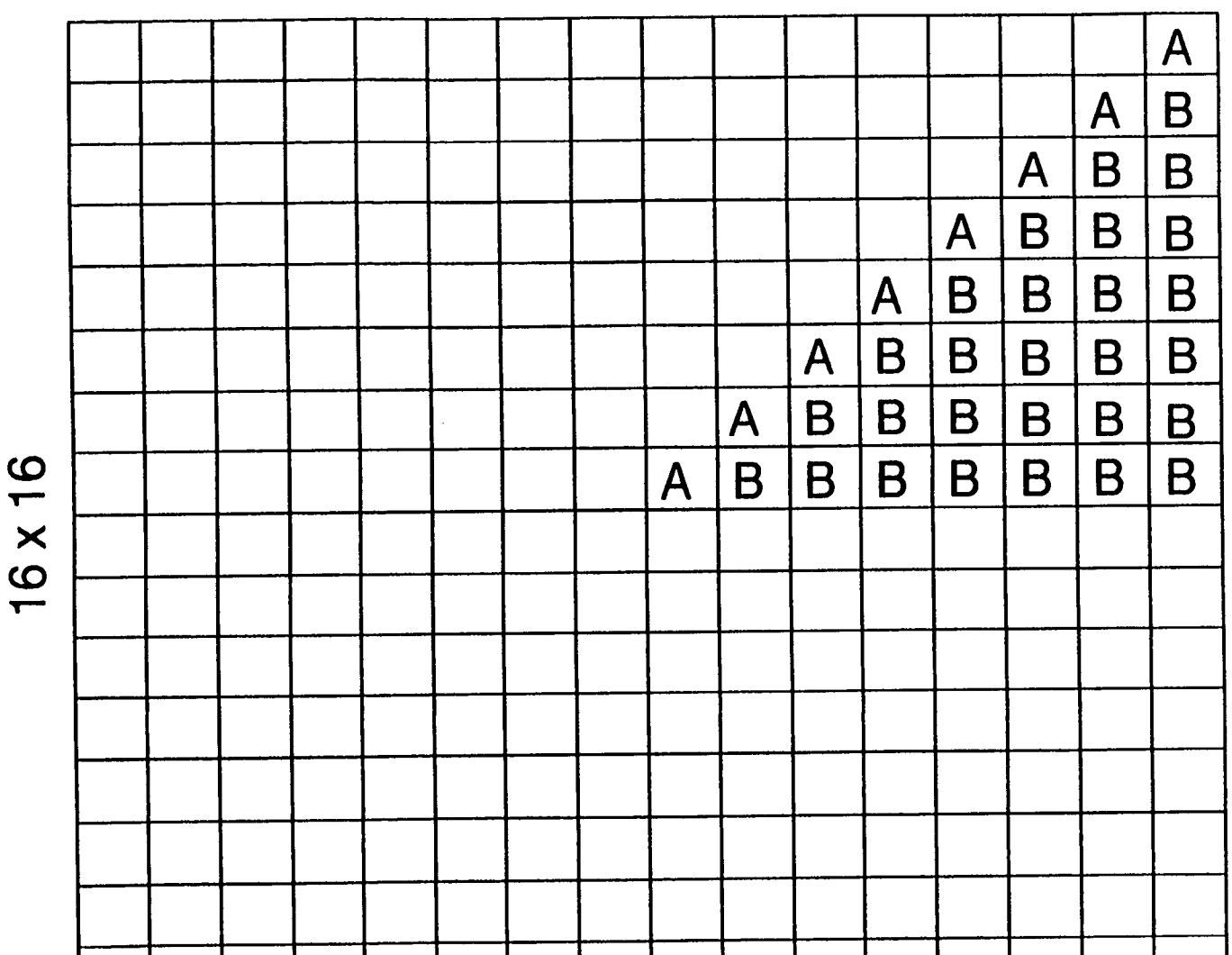

Figure 3-2. Definition of repository cells and groups

container internal temperature are calculated as functions 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 rates are estimated. The container temperature, corrosion penetration depth, and area penetrated by corrosion are then used either to estimate the release for a single radionuclide or to assess the structural integrity of the container. The residual strengths of buckling, fracture, and yield are then compared with a deterministic seismic-induced stress to determine if a mechanical failure occurs. Note that in the current version of the code, mechanical failure does not affect the release rate calculation. The above process is repeated incrementally until the end simulation time has been reached. Selected calculational results such as the time-to-wetting and time-to-failure are stored in output files.

Data are read in from an input deck and written to several output files (simple.out; main.out; summary.out; and mechanical.out). Brine.f is the main program that controls the flow of all calculations. Subroutines are in files: input.f, lsodes.f, ode.f, mech.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. These common blocks are used to store data that do not generally change. This storage reduces the potential for errors in the input deck. The functions of these files are summarized in Table 3-1.

Table 3-1. Function of SCCEX files

Name	Function
brine.f	controls the flow of all calculations
input.f	read in data from UNIX standard input format
lsodes.f	package for solving ordinary differential equations
ode.f	routines for solving ordinary differential equations
mech.f	routine to determine mechanical failure
subroutines.f	this file contains several important subroutines: 1. rate: calculate derivatives for the main calculations. 2. derivs: calculate derivatives for the repository source. 3. green: calculate Green's function for parallel piped heat source. 4. power: calculate the power in J/yr per metric ton of initial metal. 5. corrode: calculate the corrosion rate and corrosion potential. 6. lint: perform linear interpolation 7. block data a: initialize vapor pressure arrays 8. block data b: data for power generation 9. function erf: calculate error function 10. ratint: interpolate rate data 11. drip: calculate flow rate of water on the container as a function of time. 12. release: calculate derivative for radionuclide release.
ecorr.f	corrosion potential variables (common block)
hist.f	time history variables and number of print time steps (parameter statement)
solve.f	variables pertinent to numerical solvers (common block)
vapor.f	vapor pressure information (parameter statement)
watt.f	thermal loading data (parameter statement)
bulk.f	common block and parameter statement

3.3 SCCEX CODE COMPILATION AND LINKING

SCCEX code is written in standard FORTRAN 77 with real*8 (double precision) variables. On the Sun workstation platform or any UNIX operating system, to compile and link the SCCEX code, the easiest way is to create a makefile. The current makefile used on a Sun workstation is shown in Table 3-2.

Table 3-2. Makefile for SCCEX code

```
brine.e   :  brine.o ode.o  input.o subroutines.o lsodes.o mech.o
             f77 -w -O4  -o brine.e brine.o ode.o input.o subroutines.o mech.o lsodes.o
brine.o   :  brine.f bulk.f hist.f ecorr.f solve.f
             f77 -w -O4 -c    brine.f
ode.o     :  ode.f
             f77 -w -O4 -c  ode.f
input.o   :  input.f bulk.f hist.f ecorr.f solve.f
             f77 -w -O4 -c  input.f
subroutines.o  :        subroutines.f bulk.f hist.f ecorr.f solve.f
             f77 -w -O4 -c  subroutines.f
lsodes.o  :  lsodes.f
             f77 -w -O4 -c  lsodes.f
mech.o       :      mech.f bulk.f
             f77 -w -O4 -c  mech.f
```

In the make file, -w is used to suppress warning message, -O4 is used to optimize the code using the optimization level 4, -o is used to name the executable file, brine.e, and -c is used to compile without linking.

3.4 HARDWARE REQUIREMENTS AND EXECUTION PROCEDURE

The SCCEX code was originally designed to run on any platform supporting standard FORTRAN 77. SCCEX consists of about 8,186 lines of code. The largest five arrays used in SCCEX are 300×100 in size; the rest of the arrays are vectors that are less than 1000 in size. Therefore, total disk space required for SCCEX should be less than 1.5 Mb.

Before running SCCEX, two steps must be taken. The first step consists of removal of any files that may conflict with the SCCEX system output file names. Secondly, the input file must be prepared for the run of interest.

To execute the SCCEX code on a UNIX system, the following command statement can be executed:

```
%brine.e  < input filename  > output filename
```

3.5 SENSITIVITY IN NUMERICAL CALCULATIONS—NUMERICAL OSCILLATIONS

The SCCEX code can experience numerical difficulties with the water balance equations (wetted area and salinity) on the container surface. The numerical problems tend to first express themselves as oscillations in the wetted area on the container surface. The numerical difficulties arise from the rapid rate of water vapor diffusion (evaporation rate) near the boiling point of water. The analytical solution for water vapor diffusion used in the SCCEX code is:

$$N_{water} = \frac{cD\tau\phi}{(1 - X_{water})} \nabla X_{water}. \qquad (3\text{-}1)$$

Note that as the mole fraction of water vapor (X_{water}) goes to one near the boiling point, the diffusion and evaporation rate go to infinity. Unfortunately, during initial wetting, the mole fraction of water vapor is always just barely below one; leading to numerical problems.

As the system cools, the vapor pressure of water drops below one and the numerical solution becomes more stable. Because the code includes the effect of salinity on water vapor pressure, the unstable region is extended over about an 8° temperature range for a sodium chloride salt (i.e., NaCl causes about an 8° increase in boiling point). Once the container surface temperature drops out of the critical range, the oscillations tend to decrease.

Any code solving systems of non-linear equations can be subject to numerical difficulties depending upon the parameters given the solver. Generally, the numerical problems can be conquered by sufficient lowering of the numerical tolerances (relative and absolute error epsilons), however this has the disadvantage of extending run times to intolerable lengths, particularly in probabilistic studies such as were performed for the SCCEX report (Sridhar et al., 1993).

A study was performed (see Appendix B) to determine the values of relative and absolute error to be used in production runs with the SCCEX code. In the study, the influence of relative error and absolute error tolerances on wetting, failure, and leachate generation times was examined. Based on this study, error tolerances were chosen that struck a balance between rapid execution times and accuracy as measured by wetting, failure, and leachate generation times.

The numerical solver default parameters chosen represent a compromise and are not intended to eliminate all numerical oscillations. Additionally, it was impractical to study every parameter combination which could be generated in the probabilistic simulation. We believe the default parameters chosen represent a judicious balance between accuracy and run time constraints. An important consideration is that excessive run times allow for fewer Monte-Carlo realizations, fewer calculational cells, and therefore higher statistical and spatial error. However, any future user of the code needs to be aware of this problem, and it is highly recommended that they check their solutions to see if they are acceptable regarding oscillatory behavior.

3.6 IMPLICATIONS OF NUMERICAL PROBLEMS FOR RESULTS REPORTED IN THE SCC REPORT

Usually, the observed numerical oscillations have no impact on wetting or leachate generation times and a minor influence on container failure time. The simulations reported in the SCCEX report (CNWRA 94-003) all use the thermodynamic initial wetting option with a switch to full solution at 1 percent water coverage. The thermodynamic wetting option has fewer numerical problems and thus initial wetting time does not generally vary because of numerical errors. The solver shifts from thermodynamic wetting to a full solution when 1 percent of the container surface is covered with water. Depending upon solver tolerances and the input data, oscillations in the solution can develop at this point. Over time, the container cools and the oscillations generally disappear. Because the oscillations tend to disappear with time, the leaching time usually is not sensitive to the numerical errors. Because the oscillations change the salinity in the water, the corrosion rate and therefore failure time can be changed by the oscillations. In our experience, with the tolerance parameters used in the SCCEX report, the numerical error in the container failure time is small.

The SCCEX code can also be used to examine wetting and water chemistry on the container surface in more detail. For example, the code allows for the input of specific infiltration/dripping events on the container surface. However, a detailed, time dependent study of wetted area and water chemistry generally requires tighter specification of numerical tolerances. Appendix B gives some examples of tolerances required to avoid oscillations in wetted area for the baseline case. It should be noted that the results given in the appendix may be somewhat different from the results produced by the latest version of the SCCEX code due to the correction of several errors in the code. Although the new modifications result in quantitative differences, the qualitative results of the sensitivity analysis are unchanged.

3.7 FUTURE CONSIDERATIONS TO REDUCE NUMERICAL PROBLEMS

The numerical performance of the code could be improved by:

(i) Replace the diffusion equation used in the SCCEX code with a new, recently developed (Lichtner and Walton, in preparation), analytical solution incorporating a combination of Fick's and Darcy's laws. The newer solution eliminates the problem of infinite evaporation rates at a mole fraction of one and should therefore be more stable numerically.

(ii) Additional programming and development time could be expended to make the code more user friendly (i.e., the code could make more numerical choices without user input).

(iii) Lower values could be used for tortuosity in the rock. Current thinking[1] is that the water vapor diffusion parameters (Cragnolino et al., 1994) may be too high by perhaps 1–3 orders of magnitude. Based upon experience, most of the numerical problems disappear when diffusion/evaporation rates are slower.

---

[1] Lichtner, P., and J. Walton. 1995. *Quasi-Steady State Model for Coupled Liquid, Vapor, and Heat Transport: Application to Yucca Mountain Near Field.* Submitted for publication.

(iv) It is possible that more robust solvers could be found, however the code already uses two of the best ODE solvers available.

3.8 USER SUPPORT

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Southwest Research Institute
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Phone: (210) 522-6084

4 INSTRUCTIONS FOR INPUT DATA

4.1 OVERVIEW

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, 1988). Detailed discussion for the input data selected in this report have been summarized by Cragnolino et al. (1994).

In the following subsections, the required input data for simulation time and reference container geometry, thermal model, environmental model, release rate and solver parameters, corrosion model, and mechanical model will be briefly discussed. In addition, the baseline input data selected will also be illustrated. Input variables are separated by commas. Note that this input file is read in a free-format fashion. Text following the exclamation point is treated as a comment. Comments must appear on the same line as the exclamation point. The same format is used for the other subsections.

4.2 SIMULATION TIME AND REFERENCE CONTAINER GEOMETRY INPUT

In the input file, the first block of data describes the simulation and reference container geometry information as follows:

Line No.

1 Title line for this input file
2 Total simulation time (in yr)
  - Variable *tend*
3 Container x,y,z location (in m), number of cells (must be a power of 4)
  - Variables *x, y, z, ncell*
4 Container length (*l*), container radius (*r*1), borehole radius+gap (*r*2), outer boundary (*r*3) (all in meters)
  - Variables *rlen, r*1, *r*2, *r*3
5 Container thickness (in m)
  - Variable *cthick*

For the baseline case, this block of data are listed as follows:

Line No.

1 This is the Brine or SCCEX code input file ! title line
2 1000. ! total simulation time
3 0., 0., 0., 4 ! container x,y,z location, number of cells
4 4.76, 0.33, 0.34, 5.0 !container length, container radius, borehole radius, outer boundary
5 0.01 ! container thickness in m

4.3 THERMAL MODEL INPUT

The second block of data describes the thermal model as follows:

Line No.

6 Title line for thermal input

7 Initial power density (in J/yr/m^2)
- Variable *powden*

8 Metric ton initial heavy metal (MTIHM) total (in tons), MTIHM per container or canister (in tons), age of fuel (in yr)
- Variables *tons, canld, age*

9 Thermal conductivity of rock (κ_r), packing (κ_p), container or canister (in J/yr/m/K)
- Variables *tkr, tkp, tk*

10 Volumetric heat capacity for rock (ρC_p), packing, container or canister (in J/m^3/K)
- Variables *rhocpr, rhocpp, rhocpc*

11 Initial temperature (in °C) and vertical extent of repository (in meters)
- Variables *tzero, vert*

For the baseline case, this block of data is listed as follows:

Line No.

6 Temperature Parameters

7 4.44473e8 ! initial power density in J/yr/m^2

8 70000., 2.3, 10. ! metric ton initial heavy metal total, MTIHM can, age of fuel

9 5.68e7, 3.787e7, 3.26e6 ! J/yr/m/K thermal conductivity for rock, packing, can

10 2.4e6, 1.2e6, 1.2e6 ! rho*Cp (volumetric heat capacity of rock) in J/m^3/K, rock, packing, can

11 23., 4.0 ! initial temperature and vertical extent of repository

4.4 ENVIRONMENTAL MODEL INPUT

The third block of data describes the environmental model as follows:

Line No.

12 Title line for environmental model input

13 Diffusive coefficient (D) of water vapor in air (in m^2/yr), reference temperature (in °C), tortuosity factor (τ) for rock and packing
- Variables *d, tdiff, taur, taup*

14 Porosity for rock (ϕ_r), porosity for packing (ϕ_p), liquid water film thickness formed on the surface of container
- Variables *phir, phip, delta* (in m)

15 The number of time and drip rate pairs
- Variable *ndrip*

16 Time in years, drip rate (in m/yr)
- Variables *qtime(i), qdrip(i)*

17 Time in years, drip rate (in m/yr)
- Variables *qtime(i), qdrip(i)*

18 Time in years, drip rate (in m/yr)
- Variables *qtime(i), qdrip(i)*

19 Time in years, drip rate (in m/yr)
- Variables *qtime(i), qdrip(i)*

20 Time in years, drip rate (in m/yr)
- Variables *qtime(i), qdrip(i)*

21 Time in years, drip rate (in m/yr)
- Variables *qtime(i), qdrip(i)*

22 Salt (in Kg/m^3), scale (in Kg/m^3)
- Variables *salt, scale*

23 Scale factor for vapor pressure lowering relative to NaCl solution
- Variable *bfact*

24 Initial salt amount (in Kg), initial scale amount (in Kg)
- Variables *dsalt, dscale*

25 Model selection (0=> no umbrella, 1=> umbrella effect), funnel area for capture of Darcy flow onto container (in m^2)
- Variables *idrip, dfrac*

26 Umbrella edge thickness (in m), umbrella edge temperature (in °C), range of temperature (in °C)
- Variables *slice, tenhan, tslop*

27 Atmospheric pressure at Yucca Mt. repository level (in atm)
- Variable *pref*

For the baseline case, this block of data is listed as follows:

Line No.	
12	Evaporation Parameters
13	962., 59., 1.0, 1.0 !diffusive coef. (m^2/yr), reference temp. (°C), tortuosity for rock and packing
14	0.12, 0.12, 2.e-3 ! porosity for rock, porosity for packing, water film thick (m)
15	6 ! ndrip, the number of time, drip rate pairs
16	0., 1.e-3 ! time in yr, drip rate in m/yr
17	100., 1.e-3 ! time in yr, drip rate in m/yr
18	400., 1.e-3 ! time in yr, drip rate in m/yr
19	3000., 1.e-3 ! time in yr, drip rate in m/yr
20	8000., 1.e-3 ! time in yr, drip rate in m/yr
21	100000., 1.e-3 ! time in yr, drip rate in m/yr
22	0.0613, 0.2121 ! salt (kg/m^3), scale (kg/m^3)
23	1.0 ! bfact, scale factor for vapor pressure lowering relative to NaCl solution
24	0.1, 0.0 ! initial salt (kg), initial scale (kg)
25	1, 1.0 ! idrip (0=> no umbrella, 1=> umbrella effect), dfrac in m^2 (fraction of Darcy flux)
26	20., 95, 2. ! umbrella edge thickness (m), umbrella edge temp. (°C), range of temp. (°C)
27	0.895 ! atmospheric pressure (atm)

4.5 RELEASE RATE AND SOLVER PARAMETERS INPUT

The fourth block of data describes the release rate and solver parameters as follows:

Line No.

28 Spent fuel alteration rate/yr (alt), radioactive decay rate/yr (λ)
- Variables *alt, rlam*

29 Initial time step (in yr), max time step (in yr), constant for selecting solver
0= > full equilibrium (Lsode), 1= > local equilibrium (ODE)
Variables *dtini, dtmax, isolve*

30 Relative error, absolute error for Lsode solver
- Variables *errrel, errabs*
Variables not used but will be enhanced later)

31 Evap/Qin factor (variable for future enhancement), fraction of maximum surface water coverage before full evaporation occurs (below this amount, local equilibrium is assumed)
- Variables *junk, amtund*

For the baseline case, this block of data is listed as follows:

Line No.

28 1.e-3, 1.39e-4 ! alt, lambda (release rate parameters)
29 1.e-3, 1.e0, 1 ! initial time step, max time step, 0= > full (Lsode), 1= > local equilibrium
30 1.e-5, 1.e-5 ! relative error, absolute error (Lsode)
31 10., 0.01 ! Evap/Qin factor, Vwater/Vcrit factor to switch from local equilibrium

4.6 CORROSION MODEL INPUT

The fifth block of data describes the corrosion model as follows:

Line No.

32 Title line for corrosion model

33 Beta kinetics parameter for oxygen (β_{O_2}) and water reduction reactions (β_{H_2O})
- Variables *betaox, betahy*

34 Rate constant for oxygen and water reduction reactions (k_{H_2O}) [all in (C m)/(mole yr)], activation energy for oxygen and water rate constant (J/mole)
- Variables *rkox, rkhy, gox, ghy*

35 Current density for air/steam, active current density (all in C/m^2/yr)
- Variables *curair, curact*

36 Passive current density (in C/m^2/yr), temperature constant for first-order, temperature constant for second-order
- Variables *aa(1), aa(2), aa(3)*

37 Linear interpolation factor for using passive or active current density [0= > (passive), 1= > (active)], constants for future enhancement
-Variables *bb(1), bb(2), bb(3), bb(4), bb(5), bb(6)*

38 Nitrate/chloride ratio, reference pH
-Variables *clrat, refph*

39 Tortuosity in scale (τ), scale porosity (ϕ)
-Variables *taus, spor*

For the baseline case, this block of data is listed as follows:

Line
No.

32 Corrosion Parameters
33 0.75, 0.5 ! beta kinetics parameter for oxygen and water
34 3.e10, 3.2, 100000., 20000. ! rate constant for oxygen and water reduction, gox, ghy
35 6.3e2, 6.3e6 ! current density for air/steam, active current density
36 6.3e4, 0.0, 0.0 ! passive current density, const., const.
37 0.0, 0.0, 0.0, 0.0, 0.0, 0.0 ! CEcrit,Counter,const.,const.,const.,const.
38 1.0, 7.0 ! nitrate/chloride ratio, reference pH
39 0.3, 0.5 ! tortuosity in scale, scale porosity

4.7 MECHANICAL MODEL INPUT

The mechanical properties of the alloys, which include yield strength (MPa), Young's modulus (MPa), Poisson's ratio, and fracture toughness ($MPa \cdot m^{1/2}$), are required by the SCCEX code. These mechanical properties will be used to compute the residual strengths (discussed in Section 2.6) that can be compared with a deterministic seismic-induced stress to determine if a mechanical failure occurs. All these mechanical properties are currently hard-coded in the SCCEX code, mechanical.f; however, this is not very convenient when different materials are used. To enhance the SCCEX code, these material properties data will also be included in the current SCCEX code input file in the future.

As discussed in the report (Cragnolino et al., 1994), five different materials were used to validate different failure mechanisms defined in the SCCEX code. Among these materials, 304L SS and alloy 825 are existing materials, and material *X*, material *Y*, and material *Z* are hypothetical materials. In this manual, 304L SS is the standard material which has yield strength of 170 MPa, Young's modulus of $1.82 \cdot 10^5$ MPa, Poisson's ratio of 0.25, and fracture toughness of 300 $MPa \cdot m^{1/2}$. The rest of the material properties can be seen in the report (Cragnolino et al., 1994).

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. For 304L SS material, several temperature-dependent functions were calculated and are listed in Table 4-1. No temperature correction was applied to fracture toughness. When using other materials, these temperature-dependent functions must also be developed.

Table 4-1. Temperature corrections for mechanical properties

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)	$1-6\times10^{-4}$ (T−20)
Poisson's ratio	$1+4\times10^{-4}$ (T−20)

5 DESCRIPTION OF OUTPUT FILES

5.1 OVERVIEW

The output files for this code include the following: sccsml.dat, mechanical.out, simple.out, main.out, summary.out, and release.out. These files are used to record the key solutions for validation, plotting, and postprocessing purposes. In the following subsections, the main purpose of each output file is discussed briefly, and a demonstration output file based on the baseline input is also included.

5.2 SCCSML.DAT

The file sccsml.dat (see Table 5-1) summarizes the weight factor, failure time, time-to-wetting, and time to leach for all calculation cells. For the later probabilistic analysis (not described here), where SCCEX code will be called several times, the results of every sccsml.dat file will be stored and will be analyzed by a postprocessing code.

Table 5-1. Output file—SCCSML.DAT

```
***** SCCEX FAILURE, WETTING, LEACHATE TIME *****
   1 ! total calculation groups
   1 ! counter
   4 ! weight factor
 775.00     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)
```

Note that explanations after the exclamation point are added to explain the results and will not be seen in the original output file. The same format is used for the other subsections.

5.3 MECHANICAL.OUT

The file mechanical.out (see Table 5-2) summarizes the temperature, wetted area, remaining thickness of the container, and leachate in each time step. This file will be read by one of the SCCEX code subroutines (mechanical) to determine if the container fails or not.

Table 5-2. Output file—MECHANICAL.OUT

```
 1  4  101 1! Counter, weight factor, total time steps, calculation cells
 1  0.100E-04  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
```

Table 5-2. Output file—MECHANICAL.OUT (Cont'd)

```
*
*7-72 or 60-710 years data
*
 73  0.720E+03  0.965E+02  0.998E-02  0.000E+00  0.000E+00
 74  0.730E+03  0.963E+02  0.998E-02  0.000E+00  0.000E+00
 75  0.740E+03  0.961E+02  0.844E-02  0.444E+00  0.000E+00
 76  0.750E+03  0.959E+02  0.605E-02  0.448E+00  0.000E+00
 77  0.760E+03  0.958E+02  0.369E-02  0.452E+00  0.000E+00
 78  0.770E+03  0.956E+02  0.129E-02  0.457E+00  0.000E+00
 79  0.780E+03  0.954E+02  0.000E+00  0.461E+00  0.000E+00
 80  0.790E+03  0.952E+02  0.000E+00  0.465E+00  0.000E+00
 81  0.800E+03  0.951E+02  0.000E+00  0.469E+00  0.000E+00
 82  0.810E+03  0.949E+02  0.000E+00  0.473E+00  0.000E+00
 83  0.820E+03  0.947E+02  0.000E+00  0.477E+00  0.000E+00
 84  0.830E+03  0.945E+02  0.000E+00  0.481E+00  0.000E+00
 85  0.840E+03  0.944E+02  0.000E+00  0.485E+00  0.000E+00
 86  0.850E+03  0.942E+02  0.000E+00  0.489E+00  0.000E+00
 87  0.860E+03  0.941E+02  0.000E+00  0.493E+00  0.000E+00
 88  0.870E+03  0.939E+02  0.000E+00  0.497E+00  0.000E+00
 89  0.880E+03  0.937E+02  0.000E+00  0.501E+00  0.000E+00
 90  0.890E+03  0.936E+02  0.000E+00  0.505E+00  0.000E+00
 91  0.900E+03  0.934E+02  0.000E+00  0.509E+00  0.000E+00
 92  0.910E+03  0.933E+02  0.000E+00  0.514E+00  0.000E+00
 93  0.920E+03  0.931E+02  0.000E+00  0.519E+00  0.000E+00
 94  0.930E+03  0.930E+02  0.000E+00  0.526E+00  0.000E+00
 95  0.940E+03  0.928E+02  0.000E+00  0.527E+00  0.000E+00
 96  0.950E+03  0.927E+02  0.000E+00  0.531E+00  0.000E+00
 97  0.960E+03  0.925E+02  0.000E+00  0.535E+00  0.000E+00
 98  0.970E+03  0.924E+02  0.000E+00  0.539E+00  0.000E+00
 99  0.980E+03  0.922E+02  0.000E+00  0.543E+00  0.000E+00
100  0.990E+03  0.921E+02  0.000E+00  0.547E+00  0.000E+00
101  0.100E+04  0.919E+02  0.000E+00  0.551E+00  0.000E+00
```

5.4 SIMPLE.OUT

The file simple.out (see Table 5-3) is an output file designed for plotting purposes. Data of several important parameters, which include the temperature at canister surface, vapor pressure, and evaporation rate, can be plotted as functions of time.

Table 5-3. Output file—SIMPLE.OUT

```
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., out temp., temp. diff., vapor pressure inside,
vapor pressure outside, 0.75*vapin, evaporation rate, evaporation rate)
```

Table 5-3. Output file—SIMPLE.OUT (Cont'd)

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
*								
* 60-710 years data								
*								
7.20E+02	9.65E+01	8.86E+01	7.86E+00	8.81E−01	6.59E−01	6.61E−01	2.54E+00	2.57E−01
7.30E+02	9.63E+01	8.85E+01	7.78E+00	8.75E−01	6.57E−01	6.56E−01	2.22E+00	2.25E−01
7.40E+02	9.61E+01	8.84E+01	7.70E+00	8.69E−01	6.54E−01	6.52E−01	2.00E+00	2.02E−01
7.50E+02	9.59E+01	8.83E+01	7.62E+00	8.63E−01	6.51E−01	6.47E−01	1.82E+00	1.85E−01
7.60E+02	9.58E+01	8.82E+01	7.55E+00	8.58E−01	6.49E−01	6.43E−01	1.68E+00	1.71E−01
7.70E+02	9.56E+01	8.81E+01	7.47E+00	8.52E−01	6.46E−01	6.39E−01	1.57E+00	1.59E−01
7.80E+02	9.54E+01	8.80E+01	7.40E+00	8.47E−01	6.44E−01	6.35E−01	1.47E+00	1.49E−01
7.90E+02	9.52E+01	8.79E+01	7.33E+00	8.41E−01	6.41E−01	6.31E−01	1.38E+00	1.40E−01
8.00E+02	9.51E+01	8.78E+01	7.26E+00	8.36E−01	6.39E−01	6.27E−01	1.31E+00	1.32E−01
8.10E+02	9.49E+01	8.77E+01	7.19E+00	8.31E−01	6.36E−01	6.23E−01	1.24E+00	1.26E−01
8.20E+02	9.47E+01	8.76E+01	7.12E+00	8.25E−01	6.34E−01	6.19E−01	1.18E+00	1.20E−01
8.30E+02	9.45E+01	8.75E+01	7.05E+00	8.20E−01	6.31E−01	6.15E−01	1.13E+00	1.14E−01
8.40E+02	9.44E+01	8.74E+01	6.99E+00	8.15E−01	6.29E−01	6.12E−01	1.08E+00	1.09E−01
8.50E+02	9.42E+01	8.73E+01	6.93E+00	8.10E−01	6.26E−01	6.08E−01	1.03E+00	1.04E−01
8.60E+02	9.41E+01	8.72E+01	6.87E+00	8.06E−01	6.24E−01	6.04E−01	9.88E−01	1.00E−01
8.70E+02	9.39E+01	8.71E+01	6.80E+00	8.01E−01	6.22E−01	6.01E−01	9.49E−01	9.61E−02
8.80E+02	9.37E+01	8.70E+01	6.75E+00	7.96E−01	6.19E−01	5.97E−01	9.12E−01	9.24E−02
8.90E+02	9.36E+01	8.69E+01	6.69E+00	7.91E−01	6.17E−01	5.93E−01	8.78E−01	8.90E−02
9.00E+02	9.34E+01	8.68E+01	6.63E+00	7.87E−01	6.14E−01	5.90E−01	8.46E−01	8.57E−02
9.10E+02	9.33E+01	8.67E+01	6.57E+00	7.82E−01	6.12E−01	5.86E−01	8.16E−01	8.27E−02
9.20E+02	9.31E+01	8.66E+01	6.52E+00	7.77E−01	6.10E−01	5.83E−01	7.88E−01	7.99E−02
9.30E+02	9.30E+01	8.65E+01	6.47E+00	7.73E−01	6.07E−01	5.80E−01	7.62E−01	7.72E−02
9.40E+02	9.28E+01	8.64E+01	6.41E+00	7.69E−01	6.05E−01	5.77E−01	7.39E−01	7.49E−02
9.50E+02	9.27E+01	8.63E+01	6.36E+00	7.65E−01	6.03E−01	5.73E−01	7.17E−01	7.27E−02
9.60E+02	9.25E+01	8.62E+01	6.31E+00	7.60E−01	6.00E−01	5.70E−01	6.97E−01	7.06E−02
9.70E+02	9.24E+01	8.61E+01	6.26E+00	7.56E−01	5.98E−01	5.67E−01	6.77E−01	6.86E−02
9.80E+02	9.22E+01	8.60E+01	6.21E+00	7.52E−01	5.96E−01	5.64E−01	6.58E−01	6.67E−02
9.90E+02	9.21E+01	8.59E+01	6.16E+00	7.48E−01	5.93E−01	5.61E−01	6.40E−01	6.49E−02
1.00E+03	9.19E+01	8.58E+01	6.11E+00	7.44E−01	5.91E−01	5.58E−01	6.21E−01	6.30E−02

5.5 MAIN.OUT

The file main.out (see Table 5-4) is an output file designed for plotting purposes. Data of several important parameters, which include the volume of water, kg of NaCl, corrosion depth, effluent drip rate, and drip rate, etc., can be plotted as functions of time.

Table 5-4. 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-05  0.00E+00  1.00E-01  2.40E-13  0.00E+00  0.00E+00  2.75E+01  2.40E-08  -9.00E+00
1.45E+02  0.00E+00
1.00E+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+00
2.00E+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  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+00
4.00E+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+00
5.00E+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+00
*
* 60-710 years data
*
7.20E+02  0.00E+00  3.26E-01  1.73E-05  0.00E+00  7.82E-01  2.75E+01  2.40E-08  -9.00E+00
9.65E+01  1.00E-03
7.30E+02  0.00E+00  3.27E-01  1.75E-05  0.00E+00  7.84E-01  2.75E+01  2.40E-08  -9.00E+00
9.63E+01  1.00E-03
7.40E+02  8.88E-04  3.27E-01  1.56E-03  0.00E+00  7.86E-01  2.69E+01  2.40E-04  1.84E-01
9.61E+01  1.00E-03
7.50E+02  8.97E-04  3.28E-01  3.95E-03  0.00E+00  7.88E-01  2.68E+01  2.40E-04  1.84E-01
9.59E+01  1.00E-03
7.60E+02  9.05E-04  3.28E-01  6.31E-03  0.00E+00  7.91E-01  2.66E+01  2.40E-04  1.84E-01
9.58E+01  1.00E-03
7.70E+02  9.13E-04  3.29E-01  8.71E-03  0.00E+00  7.93E-01  2.65E+01  2.40E-04  1.84E-01
9.56E+01  1.00E-03
7.80E+02  9.21E-04  3.30E-01  1.00E-02  0.00E+00  7.95E-01  2.64E+01  2.40E-08  -9.00E+00
9.54E+01  1.00E-03
7.90E+02  9.30E-04  3.30E-01  1.00E-02  0.00E+00  7.97E-01  2.62E+01  2.40E-08  -9.00E+00
9.52E+01  1.00E-03
8.00E+02  9.38E-04  3.31E-01  1.00E-02  0.00E+00  7.99E-01  2.61E+01  2.40E-08  -9.00E+00
9.51E+01  1.00E-03
8.10E+02  9.47E-04  3.32E-01  1.00E-02  0.00E+00  8.01E-01  2.59E+01  2.40E-08  -9.00E+00
9.49E+01  1.00E-03
8.20E+02  9.54E-04  3.32E-01  1.00E-02  0.00E+00  8.03E-01  2.58E+01  2.40E-08  -9.00E+00
9.47E+01  1.00E-03
8.30E+02  9.62E-04  3.33E-01  1.00E-02  0.00E+00  8.05E-01  2.57E+01  2.40E-08  -9.00E+00
9.45E+01  1.00E-03
8.40E+02  9.70E-04  3.33E-01  1.00E-02  0.00E+00  8.08E-01  2.56E+01  2.40E-08  -9.00E+00
9.44E+01  1.00E-03
8.50E+02  9.78E-04  3.34E-01  1.00E-02  0.00E+00  8.10E-01  2.55E+01  2.40E-08  -9.00E+00
9.42E+01  1.00E-03
8.60E+02  9.86E-04  3.35E-01  1.00E-02  0.00E+00  8.12E-01  2.53E+01  2.40E-08  -9.00E+00
9.41E+01  1.00E-03
```

Table 5-4. Output file—MAIN.OUT (Cont'd)

```
8.70E+02 9.93E-04 3.35E-01 1.00E-02 0.00E+00 8.14E-01 2.52E+01 2.40E-08 -9.00E+00
9.39E+01 1.00E-03
8.80E+02 1.00E-03 3.36E-01 1.00E-02 0.00E+00 8.16E-01 2.51E+01 2.40E-08 -9.00E+00
9.37E+01 1.00E-03
8.90E+02 1.01E-03 3.36E-01 1.00E-02 0.00E+00 8.18E-01 2.50E+01 2.40E-08 -9.00E+00
9.36E+01 1.00E-03
9.00E+02 1.02E-03 3.37E-01 1.00E-02 0.00E+00 8.20E-01 2.49E+01 2.40E-08 -9.00E+00
9.34E+01 1.00E-03
9.10E+02 1.03E-03 3.38E-01 1.00E-02 0.00E+00 8.22E-01 2.47E+01 2.40E-08 -9.00E+00
9.33E+01 1.00E-03
9.20E+02 1.04E-03 3.38E-01 1.00E-02 0.00E+00 8.25E-01 2.46E+01 2.40E-08 -9.00E+00
9.31E+01 1.00E-03
9.30E+02 1.05E-03 3.39E-01 1.00E-02 0.00E+00 8.27E-01 2.44E+01 2.40E-08 -9.00E+00
9.30E+01 1.00E-03
9.40E+02 1.05E-03 3.40E-01 1.00E-02 0.00E+00 8.29E-01 2.44E+01 2.40E-08 -9.00E+00
9.28E+01 1.00E-03
9.50E+02 1.06E-03 3.40E-01 1.00E-02 0.00E+00 8.31E-01 2.43E+01 2.40E-08 -9.00E+00
9.27E+01 1.00E-03
9.60E+02 1.07E-03 3.41E-01 1.00E-02 0.00E+00 8.33E-01 2.41E+01 2.40E-08 -9.00E+00
9.25E+01 1.00E-03
9.70E+02 1.08E-03 3.41E-01 1.00E-02 0.00E+00 8.35E-01 2.40E+01 2.40E-08 -9.00E+00
9.24E+01 1.00E-03
9.80E+02 1.09E-03 3.42E-01 1.00E-02 0.00E+00 8.37E-01 2.39E+01 2.40E-08 -9.00E+00
9.22E+01 1.00E-03
9.90E+02 1.09E-03 3.43E-01 1.00E-02 0.00E+00 8.39E-01 2.38E+01 2.40E-08 -9.00E+00
9.21E+01 1.00E-03
1.00E+03 1.10E-03 3.43E-01 1.00E-02 0.00E+00 8.41E-01 2.37E+01 2.40E-08 -9.00E+00
9.19E+01 1.00E-03
```

5.6 SUMMARY.OUT

The file summary.out (see Table 5-5) summarizes some of the main results, which are similar to those in file sccsml.dat.

Table 5-5. Output file—SUMMARY.OUT

```
1  101  4  !calc. cell, pts/cell, tot. cell
4  0.571E+03  0.571E+03  0.731E+03  0.963E+02  0.100E+04  0.000E+00  0.780E+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)
```

5.7 RELEASE.OUT

The file release.out (see Table 5-6) summarizes radionuclide release information. Data of this file can be plotted as a function of time to study the effect of input parameters.

Table 5-6. 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
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
*
* 60-710 years data
*
7.20E+02  0.00E+00  9.05E-01  0.00E+00  0.00E+00  0.00E+00
7.30E+02  0.00E+00  9.04E-01  0.00E+00  0.00E+00  0.00E+00
7.40E+02  0.00E+00  9.02E-01  0.00E+00  0.00E+00  0.00E+00
7.50E+02  0.00E+00  9.01E-01  0.00E+00  0.00E+00  0.00E+00
7.60E+02  0.00E+00  9.00E-01  0.00E+00  0.00E+00  0.00E+00
7.70E+02  0.00E+00  8.98E-01  0.00E+00  0.00E+00  0.00E+00
7.80E+02  0.00E+00  8.97E-01  1.67E-04  0.00E+00  0.00E+00
7.90E+02  0.00E+00  8.87E-01  9.13E-03  0.00E+00  0.00E+00
8.00E+02  0.00E+00  8.77E-01  1.81E-02  0.00E+00  0.00E+00
8.10E+02  0.00E+00  8.67E-01  2.70E-02  0.00E+00  0.00E+00
8.20E+02  0.00E+00  8.56E-01  3.59E-02  0.00E+00  0.00E+00
8.30E+02  0.00E+00  8.46E-01  4.47E-02  0.00E+00  0.00E+00
8.40E+02  0.00E+00  8.36E-01  5.36E-02  0.00E+00  0.00E+00
8.50E+02  0.00E+00  8.26E-01  6.24E-02  0.00E+00  0.00E+00
8.60E+02  0.00E+00  8.16E-01  7.12E-02  0.00E+00  0.00E+00
8.70E+02  0.00E+00  8.06E-01  7.99E-02  0.00E+00  0.00E+00
8.80E+02  0.00E+00  7.96E-01  8.87E-02  0.00E+00  0.00E+00
8.90E+02  0.00E+00  7.86E-01  9.74E-02  0.00E+00  0.00E+00
9.00E+02  0.00E+00  7.76E-01  1.06E-01  0.00E+00  0.00E+00
9.10E+02  0.00E+00  7.66E-01  1.15E-01  0.00E+00  0.00E+00
9.20E+02  0.00E+00  7.57E-01  1.23E-01  0.00E+00  0.00E+00
9.30E+02  0.00E+00  7.47E-01  1.32E-01  0.00E+00  0.00E+00
9.40E+02  0.00E+00  7.37E-01  1.41E-01  0.00E+00  0.00E+00
9.50E+02  0.00E+00  7.27E-01  1.49E-01  0.00E+00  0.00E+00
9.60E+02  0.00E+00  7.17E-01  1.58E-01  0.00E+00  0.00E+00
9.70E+02  0.00E+00  7.08E-01  1.66E-01  0.00E+00  0.00E+00
9.80E+02  0.00E+00  6.98E-01  1.75E-01  0.00E+00  0.00E+00
9.90E+02  0.00E+00  6.88E-01  1.83E-01  0.00E+00  0.00E+00
1.00E+03  0.00E+00  6.79E-01  1.92E-01  0.00E+00  0.00E+00
```

6 CONCLUSION

The SCCEX Computer code has been developed to demonstrate an approach for evaluating containment by a waste package and to identify those areas requiring more detailed analysis. This report presents a brief theory description of several models used in the SCCEX code. These models include the repository thermal fields, near-field environment, release rate, corrosion of container materials, and mechanical failure models. The SCCEX code structure, capability, compilation and linking, hardware requirements and installation procedure, and user support were also discussed. In addition, the baseline case input data requirements and the corresponding output files were presented. The results of an example problem using this computer code were used in support of evaluating the substantially complete containment rule for waste packages in 10 CFR Part 60 (Cragnolino et al., 1994).

To implement the SCCEX code, simplified models were used, and assumptions and approximations were made to provide a quantitative representation of the actual conditions that may be presented in an unsaturated repository site as the one modeled here. For example, a 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. Another shortcoming is that the current SCCEX code does not consider the chemistry of the final solution more rigorously [e.g., inhibiting species for localized corrosion (i.e., nitrate) as well as other anions, such as sulfate, bicarbonate, etc.]. Other limitations are discussed in the report by Cragnolino et al. (1994).

The current SCCEX code is applicable to various designs that involve different materials and failure mechanisms (Cragnolino et al., 1994). In addition, the code can be used to study the sensitivity of the input parameters and can be coupled with probabilistic analysis methods to determine if the container provides "substantially complete containment" (Cragnolino et al., 1994). The SCCEX code has provided an initial step to explore the complex problem of HLW waste containment.

7 REFERENCES

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APPENDIX

PARAMETRIC SENSITIVITY STUDY

PARAMETRIC SENSITIVITY STUDY

This appendix describes the problem setup, results, and observations of an analysis performed to determine the values of relative and absolute error tolerances to be used in production runs.

A.1 PARAMETRIC EVALUATION PROBLEM SETUP 1

A.1.1 Constant Data

- Two thousand years simulation time
- Sixteen cells
- SCP design (r = 0.33m, t = 0.01m, l = 4.76m)
- A warm container data
- Same evaporation parameters data
- Same corrosion data (new updated data)

A.1.2 Control Data

- Umbrella effect
- Solver selection - ODE (local equilibrium) or LSODES (full equilibrium)
- Relative tolerance and absolute tolerance for ODE and LSODES
- Dtini and dtmax (initial and maximum time step values) for both ODE and LSODES

The recent updated code is used to test a total of 26 examples. The selected control data for these examples are listed in Table A-1. Example one input data is listed in Table A-2.

A.2 RESULTS—OBSERVATIONS

Solver time, wetting time, and leaching time are summarized in Table A-3.

Failure time, wetting time, and leaching time are summarized in Table A-4.

A.2.1 Umbrella: With (examples 1-8) and Without (examples 9-16)

- Solver time:
  - — Difficult to determine [compare examples (1,9), (2,10), (3,11), (4,12), (5,13), (6,14), (7,15), and (8,16)]

- Failure time:

  — With/without umbrella effect produce almost the same failure time except example 7

- Wetting time:

  — With/without umbrella effect produce almost the same wetting time except examples 4 and 7

- Leaching time:

  — Same results

A.2.2 Local and Full Equilibrium: Local (examples 1-3, 9-11) and Full (examples 4-8 and 12-16)

- Solver time:

  — Difficult to determine [compare examples (1,4,5,6) and (9,12,13,14)]

- Failure time:

  — Local equilibrium produces much higher failure time than full equilibrium

- Wetting time:

  — Local equilibrium produces much higher wetting time than full equilibrium

- Leaching time:

  — Same results

A.2.3 Dtini and Dtmax

- Solver time:

  — Smaller dtini and dtmax increase both local and full solver time greatly [compare examples (1,2,3), (4,7,8), (9,10,11), and (12,15,16)]

- Failure time:

  — For either local or full equilibrium, failure time remains the same for all selected dtini and dtmax values

- Wetting time:

  — For local equilibrium (with/without umbrella effect), wetting time remains the same for all selected dtini and dtmax

— For full equilibrium with umbrella effect, wetting time remains the same

— For full equilibrium without umbrella effect, larger dtini and dtmax values (or larger relative and absolute tolerance) increase the wetting time (see example 4)

- Leaching time:

— Same results

A.2.4 Relative and Absolute Tolerances

- Solver time:

— Smaller relative and absolute tolerance increase full equilibrium solver time greatly [examples (4,5,6), and (12,13,14)].

— Smaller relative and absolute tolerance only increase local equilibrium solver time when larger dtini and dtmax values are used (see examples 1 and 9). When smaller dtini and dtmax values are used, local equilibrium solver time becomes insensitive to both relative and absolute tolerances (see examples 2, 3, 10, and 11).

- Failure time:

— With the same solver, failure time remains the same for all selected tolerances

- Wetting time:

— For full equilibrium with umbrella effect, wetting time remains the same

— For full equilibrium without umbrella effect, larger relative and absolute tolerance (or larger dtini and dtmax) increase the wetting time

- Leaching time:

— Same results

A.3 SUMMARY

- By comparing examples 4, 7, and 8: Without umbrella and full equilibrium

— Smaller solving time occurs when larger tolerances and larger dtini and dtmax are used together

— A numerical error occurs when both tolerances and dtini and dtmax become too large (check wetting time of examples 4 and 7).

- By comparing examples 1, 2, and 3: Without umbrella and local equilibrium

— With larger dtini and dtmax, smaller solving time occurs when larger tolerances are used (see example 1)

— However, when smaller dtini and dtmax are used, solving time becomes insensitive to tolerances (see examples 2 and 3)

- By comparing examples 9, 10, and 11: With umbrella and local equilibrium

  — Irregular solving time occurs when larger tolerances and larger dtini and dtmax are used together (see example 9)

  — However, when smaller dtini and dtmax are used, solving time becomes insensitive to tolerances [see examples (10,10.1) and (11,11.1)]

- Irregular (decreasing) solver time for different cells (see Table A-3):

  — Examples 5, 6, 13, and 14 all use full (Lsodes) with smaller tolerances

  — Example 9 uses local (ODE) with smaller tolerances and larger dtini and dtmax

- Irregular wetted area summarized in mechanical.out is found in several examples which are summarized in Table A-5. All these examples have larger relative and absolute tolerance and larger dtini and dtmax.

Table A-1. Sixteen examples data

No.	Umbrel Y or N	Isolve 0 or 1	Rel. Tol.	Abs. Tol.	dtini	dtmax
1	N	1	1.E-5	1.E-6	1.E-3	1.E-0
1.1	N	1	1.E-1	1.E-2	1.E-3	1.E-0
1.2	N	1	1.E-3	1.E-4	1.E-3	1.E-0
2	N	1	1.E-5	1.E-6	1.E-4	1.E-1
2.1	N	1	1.E-2	1.E-1	1.E-4	1.E-1
3	N	1	1.E-5	1.E-6	1.E-5	1.E-2
4	N	1	1.E-1	1.E-2	1.E-3	1.E-0
4.1	N	0	1.E-2	1.E-3	1.E-3	1.E-0
5	N	0	1.E-3	1.E-4	1.E-3	1.E-0
6	N	0	1.E-5	1.E-6	1.E-3	1.E-0
7	N	0	1.E-1	1.E-2	1.E-4	1.E-1
7.1	N	0	1.E-2	1.E-3	1.E-4	1.E-1
7.2	N	0	1.E-3	1.E-4	1.E-4	1.E-1
8	N	0	1.E-1	1.E-2	1.E-5	1.E-2
9	Y	1	1.E-5	1.E-6	1.E-3	1.E-0
9.1	Y	1	1.E-1	1.E-2	1.E-3	1.E-0
9.2	Y	1	1.E-5	1.E-6	1.E-4	1.E-1
10	Y	1	1.E-5	1.E-6	1.E-4	1.E-1
10.1	Y	1	1.E-1	1.E-2	1.E-4	1.E-1
11	Y	1	1.E-5	1.E-6	1.E-5	1.E-2
11.1	Y	1	1.E-1	1.E-2	1.E-5	1.E-2
12	Y	0	1.E-1	1.E-2	1.E-3	1.E-0
13	Y	0	1.E-3	1.E-4	1.E-3	1.E-0
14	Y	0	1.E-5	1.E-6	1.E-3	1.E-0
15	Y	0	1.E-1	1.E-2	1.E-4	1.E-1
16	Y	0	1.E-1	1.E-2	1.E-5	1.E-2

Table A-2. Example 1 input data

```
This is the Brine or SCCEX code input file
2000.        ! end simulation time
0., 0., 0.,  16  ! 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
4.4e8        ! initial power density in J/yr/m^2
70000., 2.3,  10.  ! metric ton initial heavy metal total, MTIHM in can, age of fuel
5.68e7,  3.79e7,  1.00e6  ! 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 (m^2/yr), tdiff (C), tau rock, tau packing
0.1, 0.1, 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-2
8000.,   1.e-2
100000., 1.e-2
0.06, 0.2  !  salt (Kg/m^3), scale (Kg/m^3)
1.0   ! bfact, scale factor for vapor pressure lowering relative to NaCl solution
0.1, 0.0  ! initial salt (Kg), initial scale (Kg)
0, 1.0   ! idrip (0=> no umbrella, 1=> umbrella effect), qfrac in m^2
10., 90, 2.  ! slice, tenhan, tslop
0.895   ! atmospheric pressure (atm)
1.e-3, 1.39e-4  ! alt, lambda
1.e-3, 1.e00, 1 ! dt ini, dtmax, isolve 0->full, 1-> local equilibrium
1.e-5, 1.e-6  ! relative error, absolute error
10., 0.1   !Evap/Qin factor, Vwater/Vcrit factor to switch from local equilibrium
Corrosion Parameters
0.25, 0.5 !        betaox, betahy
3.87e-8, 3.28, 60., 20. !        rkox, rkhy, Gox, Ghy
2.e-6, 10. !        curair, curact
2.e-4, 0.0, 0.0 !  aa(1-3)
1.268, -3.21e-3, 0.0, 0.0, 0.0, 0.0  ! bb(1-6)
1.0, 7.0  ! nitrate/cl ratio, reference pH
0.5, 0.3  ! tortuosity in scale, porosity in scale
```

Table A-3. Results comparison

No.	Sov1*	Sov2*	Sov3*	wet1#	wet2#	wet2#	lea1&	lea2&	lea3&
1	18.8	17.8	17.6	730	750	770	2000	2000	2000
1.1	9.2	9.1	9.1	730	750	770	2000	2000	2000
1.2	10.0	9.4	10.1	730	750	770	2000	2000	2000
2	72.2	71.9	77.0	730	750	770	2000	2000	2000
2.1	75.3	75.3	71.8	730	750	770	2000	2000	2000
3	697.0	697.0	696.0	730	750	770	2000	2000	2000
4	1.2	1.2	1.2	430	410	350	2000	2000	2000
4.1	1.9	1.1	1.4	710	330	670	2000	2000	2000
5	24.6	15.9	11.3	330	330	310	2000	2000	2000
6	34.6	24.9	18.7	330	330	310	2000	2000	2000
7	10.2	10.2	10.6	330	370	330	2000	2000	2000
7.1	10.7	10.7	10.7	330	330	330	2000	2000	2000
7.2	26.3	19.5	16.0	330	330	310	2000	2000	2000
8	96.0	96.2	95.7	330	330	310	2000	2000	2000
9	119.0	70.5	52.8	730	750	770	2000	2000	2000
9.1	7.4	7.4	7.3	730	750	770	2000	2000	2000
9.2	72.9	42.3	30.8	730	750	770	2000	2000	2000
10	55.0	53.9	54.5	730	750	770	2000	2000	2000
10.1	53.5	52.9	53.4	730	750	770	2000	2000	2000
11	509.0	508.0	513.0	730	750	770	2000	2000	2000
11.1	543.0	521.0	525.0	730	750	770	2000	2000	2000
12	1.0	1.0	1.0	330	330	310	2000	2000	2000
13	57.7	58.0	33.9	330	330	310	2000	2000	2000
14	72.6	63.9	58.2	330	330	310	2000	2000	2000
15	10.4	10.6	10.4	330	330	310	2000	2000	2000
16	95.8	95.5	96.7	330	330	310	2000	2000	2000

* — Solver time for different cell # — Wetting time for different cell
& — Leaching time for different cell

Table A-4. Results comparison

No.	fal1*	fal2*	fal3*	wet1#	wet2#	wet2#	lea1&	lea2&	lea3&
1	740	760	780	730	750	770	2000	2000	2000
1.1	740	760	780	730	750	770	2000	2000	2000
1.2	740	760	780	730	750	770	2000	2000	2000
2	740	760	780	730	750	770	2000	2000	2000
2.1	740	760	780	730	750	770	2000	2000	2000
3	740	760	780	730	750	770	2000	2000	2000
4	340	340	320	430	410	350	2000	2000	2000
4.1	360	360	320	710	330	670	2000	2000	2000
5	340	340	320	330	330	310	2000	2000	2000
6	340	340	320	330	330	310	2000	2000	2000
7	340	340	340	330	370	330	2000	2000	2000
7.1	340	340	320	330	330	330	2000	2000	2000
7.2	340	340	320	330	330	310	2000	2000	2000
8	340	340	320	330	330	310	2000	2000	2000
9	740	760	780	730	750	770	2000	2000	2000
9.1	740	760	780	730	750	770	2000	2000	2000
9.2	740	760	780	730	750	770	2000	2000	2000
10	740	760	780	730	750	770	2000	2000	2000
10.1	740	760	780	730	750	770	2000	2000	2000
11	740	760	780	730	750	770	2000	2000	2000
11.1	740	760	780	730	750	770	2000	2000	2000
12	340	340	320	330	330	310	2000	2000	2000
13	340	340	320	330	330	310	2000	2000	2000
14	340	340	320	330	330	310	2000	2000	2000
15	340	340	320	330	330	310	2000	2000	2000
16	340	340	320	330	330	310	2000	2000	2000

* — Solver time for different cell # — Wetting time for different cell
& — Leaching time for different cell

Table A-5. Examples with irregular wetting area data

No.	Umbrel Y or N	Isolve 0 or 1	Rel. Tol.	Abs. Tol.	dtini	dtmax
4	N	0	1.E-1	1.E-2	1.E-3	1.E-0
4.1	N	0	1.E-2	1.E-3	1.E-3	1.E-0
7	N	0	1.E-1	1.E-2	1.E-4	1.E-1
7.1	N	0	1.E-2	1.E-3	1.E-4	1.E-1
12	Y	0	1.E-1	1.E-2	1.E-3	1.E-0
13	Y	0	1.E-3	1.E-4	1.E-3	1.E-0
14	Y	0	1.E-5	1.E-6	1.E-3	1.E-0

A.4 PARAMETRIC EVALUATION PROBLEM SETUP 2

A.4.1 Constant Data

- One thousand years simulation time
- Four cells
- SCP design (r = 0.33m, t = 0.01m, l = 4.76m)
- A warm container data
- Same evaporation parameters data
- Same solver selection - ODE (local equilibrium)
- Same corrosion data

A.4.2 Control Data

- Umbrella effect
- Relative tolerance and absolution tolerance for ODE
- Dtini and dtmax (initial and maximum time step values) for ODE
- Time interval size (baseline uses 10 years)

The SCCEX code was used to test a total of 10 problems. The selected control data for these problems are listed in Table A-6. Example one (baseline case) input data is listed in Table A-7.

A.5 RESULTS SUMMARY

Solver time, failure time, and wetting time are summarized in Table A-8. The calculations show the effect of relative and absolute tolerances on oscillations in the total wetted area and salinity and the CPU times.

Table A-6. Input data summary

No.	Time Int.	Umbrel Y or N	Vwater/ Vcrit	Rel. Tol.	Abs. Tol.	dtini	dtmax
1	10	Y	0.01	1.E-3	1.E-3	1.E-3	1.E-0
2	10	Y	0.01	1.E-5	1.E-6	1.E-3	1.E-0
3	10	Y	0.01	1.E-7	1.E-8	1.E-3	1.E-0
4	10	Y	0.01	1.E-3	1.E-3	1.E-5	1.E-2
5	10	Y	0.1	1.E-3	1.E-3	1.E-3	1.E-0
6	10	Y	0.01	1.E-5	1.E-6	1.E-4	1.E-1
7	10	N	0.01	1.E-5	1.E-6	1.E-3	1.E-0
8	5	Y	0.01	1.E-5	1.E-6	1.E-4	1.E-1
9	2.5	Y	0.01	1.E-5	1.E-6	1.E-4	1.E-1
10	1	Y	0.01	1.E-5	1.E-6	1.E-4	1.E-1

Table A-7. Example 2 input data

```
This is the Brine or SCCEX code input file
1000.        ! end simulation time
0., 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/m^2
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 (m^2/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/m^3), scale (Kg/m^3)
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), qfrac in m^2
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 A-8. Results comparison

No.	CPU Thermal	CPU ODE	Time to Wet	Time to Fail	Smooth or not (Yes/No)[1]
1	5.20	9.02	735	795[2]	No[3]
2	5.28	27.7	735	775	No[3]
3	5.33	29.3[4]	735	775	Yes
4	5.25	121.0[5]	735	775	Yes
5	5.28	2.3	735	775	Yes
6	5.23	14.3	735	775	Yes
7	5.27	25.9	735	775	Yes
8	15.6[6]	14.6	732.5	777.5	Yes
9	59.6[6]	16.5	733.5	776.25	Yes
10	365.0[6]	20.3	733.5	775.5	Yes

1 Total wetted area and salinity
2 Baseline case has different failure time (795)
3 Examples 1 and 2 have some oscillations in wetted area and salinity
4 Decrease in relative and absolute tolerance will increase the CPU time
5 Decrease in dtini and dtmax will increase the CPU time
6 Reduction in the time interval will increase both CPU times especially the CPU time for calculating the thermal results