

**SEISMO VERSION 1.0—A MODULE FOR SIMULATION
OF SEISMO-MECHANICAL SCENARIOS, MODEL
DESCRIPTION, AND USER GUIDE**

Iterative Performance Assessment Phase 2

Prepared for

**Nuclear Regulatory Commission
Contract NRC-02-93-005**

Prepared by

**Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas**

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Prepared by

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ABSTRACT

This user guide describes the SEISMO code, its structures, the associated simulation model, and instructions for its use. The SEISMO code has been used in the Iterative Performance Assessment (IPA) Phase 2 exercise to simulate the effect of a seismic event on the integrity of the proposed high-level waste (HLW) repository at the Yucca Mountain site. The code models the seismic event as a random process and then assesses the consequences of the event on the HLW repository in terms of the premature release of radioactivity to the geologic media.

The SEISMO code is run under the Total-System Performance Assessment (TPA) code. SEISMO determines the time at which the waste package fails by comparing the probability associated with the acceleration needed for failure to the probability that there will be an earthquake of that magnitude within the next 10,000 yr. In the event of premature failure of the waste packages in the repository region, these data are then communicated to other modules of the TPA code.

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FOREWORD

In accordance with the provisions of the Nuclear Waste Policy Act of 1982, the Nuclear Regulatory Commission (NRC) has the responsibility of evaluating and granting a license for the first and subsequent, if any, geological repositories for high-level nuclear waste (HLW). This act was amended in 1987 to designate one site in the unsaturated region of tuffaceous rocks of Yucca Mountain in southern Nevada for detailed characterization. To meet its licensing function, the NRC will review the application submitted by the U.S. Department of Energy (DOE). The Center for Nuclear Waste Regulatory Analyses (CNWRA) at Southwest Research Institute (SwRI) is a Federally Funded Research and Development Center (FFRDC) created to support the NRC in its mission of evaluating and licensing the proposed HLW repository. One critical section of the DOE license application will deal with the assessment of the future performance of the repository system, which has to meet certain standards established by regulations.

In order to develop capabilities to review the Performance Assessment (PA) in the DOE license application, the NRC and the CNWRA are engaged in developing and applying PA methods and models to existing data. Later, at the time of the license application review, these methods may be used to conduct independent PA, if the NRC elects to do so. Because of the large space and time scales involved in estimating repository performance, mathematical models encoded as computer codes are the chosen tools for PA. The repository system consists of designed (or engineered) barriers embedded in the natural geologic setting. Estimating performance of the total system requires that the behavior of these components be projected under a variety of possible future conditions. This effort is obviously a complex task that requires a variety of calculations. The development of the SEISMO code, described in this report, is a part of the total performance assessment computer code and performs the calculations associated with the seismo-mechanical behavior of the waste packages.

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1 INTRODUCTION

1.1 REGULATORY AND TECHNICAL BACKGROUND

The Nuclear Regulatory Commission (NRC), in conjunction with the Center for Nuclear Waste Regulatory Analyses (CNWRA), is developing an independent performance assessment (PA) capability to (Codell et al., 1992):

- Aid in developing an independent understanding of the processes, conditions, and events important to predicting long-term repository performance and their relative significance in such predictions
- Provide an independent capability for reviewing U.S. Department of Energy (DOE) demonstrations of compliance with the overall system and subsystem performance objectives
- Aid in the detailed technical review of DOE iterative total-system and subsystem PAs
- Contribute to the development of guidance to the DOE on the adequacy of site characterization data and repository design, with respect to demonstrating compliance with the regulations

This independent PA capability is designed to calculate estimates of repository performance specified in the regulations. To make predictions of performance and comparisons with regulatory performance measures, the Total-System Performance Assessment (TPA) code has been developed to provide computational algorithms for estimating values of various performance measures [see Sagar and Janetzke (1993) for the description of the TPA code]. To estimate the performance measures, the TPA code contains a set of Consequence Modules (CMs) that are largely independent computational units. The SEISMO code, which is one of these CMs, is used to evaluate the consequence on the high-level waste (HLW) repository due to seismic events in the vicinity of Yucca Mountain (YM).

The primary regulations applicable to the HLW geological repository were promulgated by the NRC in 10 CFR Part 60—Disposal of High-Level Radioactive Wastes in Geologic Repositories. Two sections of 10 CFR Part 60 pertain specifically to post-closure performance. These sections include Part 60.112—Overall System Performance Objective for the Geologic Repository after Permanent Closure and Part 60.113—Performance of Particular Barriers after Permanent Closure. Part 60.112 makes reference to satisfying the generally applicable environmental standards for radioactivity established by the Environmental Protection Agency (EPA). These environmental standards were promulgated by the EPA in 40 CFR Part 191 in 1985. However, on litigation, certain provisions of these standards were remanded by a federal court. Proposed revisions of 40 CFR Part 191 were under review in early 1993. In late 1992, the U.S. Congress enacted a new law known as the Energy Policy Act, according to which the EPA will develop standards applicable specifically to YM that may be different from those in 40 CFR Part 191. However, for the development of the SEISMO code, the 1985 EPA standards are followed. The SEISMO code will be modified, as necessary, at the appropriate time to account for any changes in the EPA rule.

Three different performance measures are used in Part 191. These measures are: (i) release of radioactivity over the entire accessible environment (AE) boundary (i.e., vertical boundary at 5 km from edge of the repository integrated over areal space) cumulated over a 10,000-yr period (integrated over

time) after closure must not exceed specific limits at specified probability levels (Part 191.13—Containment Requirements), where the preferred method of representing this performance measure is through a Complementary Cumulative (Probability) Distribution Function (CCDF); (ii) dose to humans in the first 1,000-yr after repository closure must not exceed specified limit (Part 191.15—Individual Protection Requirements—this requirement is deterministic); and (iii) concentration of alpha-, beta-, and gamma-emitting radionuclides must not exceed specified limits (Part 191.16—Groundwater Protection Requirements—this requirement is deterministic). While the first performance measure is to consider all future credible scenarios, the other two apply only to undisturbed performance.

Three other performance measures are used in 10 CFR Part 60.113 to define performance of individual barriers (in contrast to the total system). These performance measures are: (i) life of the waste package must exceed specified limit [Part 60.113(a)(ii)(A)—Substantially Complete Containment Requirement], (ii) release from engineered barriers must be less than specified limits [Part 60.113(a)(1)(ii)(B)—Groundwater Release Requirement], and (iii) Groundwater Travel Time (GWTT) must be greater than specified limit [Part 60.113(a)(2)—Groundwater Travel Time Requirement].

In total, there are six distinct performance measures. In general, the TPA code must accommodate compliance determination by estimation of the three measures related to 40 CFR Part 191 and preferably, but not necessarily, the three measures related to 10 CFR Part 60.113. Figure 1-1 depicts schematically the six performance measures and lists the generic steps for their assessment. The steps for the assessment of the six performance measures include model conceptualization of process, assembly of data suitable for input to the mathematical models calculating consequences, sensitivity and uncertainty analysis, and regulatory compliance assessment. The NRC and CNWRA are developing regulatory definitions for the performance measure of 60.113 and the corresponding complementary determination methods. Performance measures computed in the Phase 2 TPA are examples to be used only to demonstrate a concept. Whether such compliance determination will be accomplished through the TPA is a decision not yet made. In any event, the Phase 2 methods are not intended to be regulatory guides and should not be taken to provide such guidance.

1.2 TOTAL-SYSTEM PERFORMANCE ASSESSMENT CODE BACKGROUND

To estimate the regulatory performance measures, the TPA code contains a set of CMs that are computationally independent units, with their coupled execution controlled by an Executive Module (Exec) (Sagar and Janetzke, 1993). The Exec acts as the manager and ensures that CMs are executed in the desired sequence and that appropriate values of the common parameters are passed to the CMs. The Exec additionally directs data flow between different subprocesses and controls their execution. Figure 1-2 shows schematically the organization of Version 2.0 of the TPA code. The shaded parts of Figure 1-2 represent the Exec. A data flow diagram, indicating inter-module communication interfaces is shown in Figure 1-3. This figure also shows all CMs of the TPA, including the SEISMO code.

1.3 PURPOSE OF SOFTWARE

The objective of the SEISMO module is to provide a computational algorithm for estimating the consequences to the HLW repository due to a seismic event, in the TPA simulations. The code describes and calculates the effects of a seismic event on the physical integrity of a waste package.

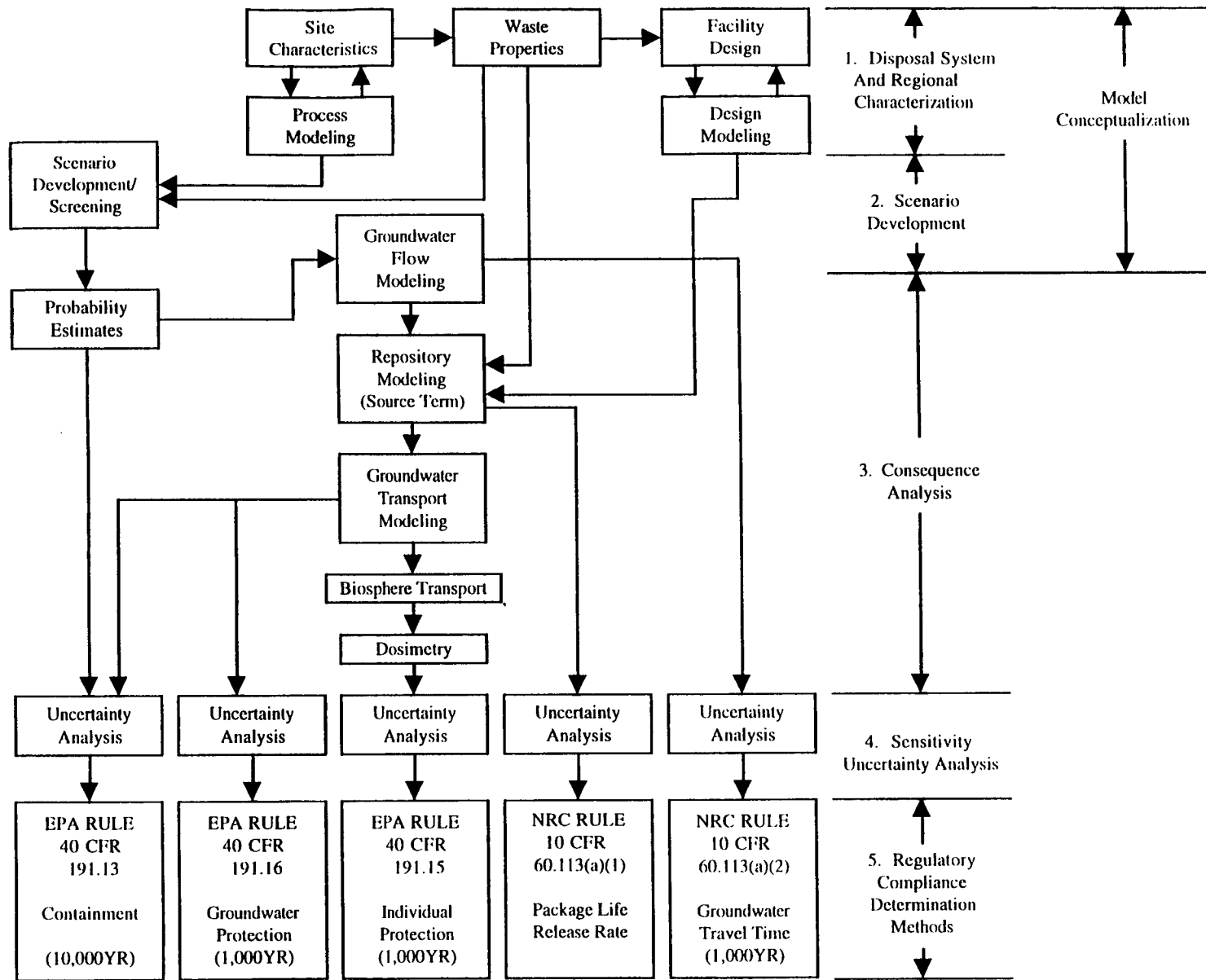


Figure 1-1. Regulatory performance measures

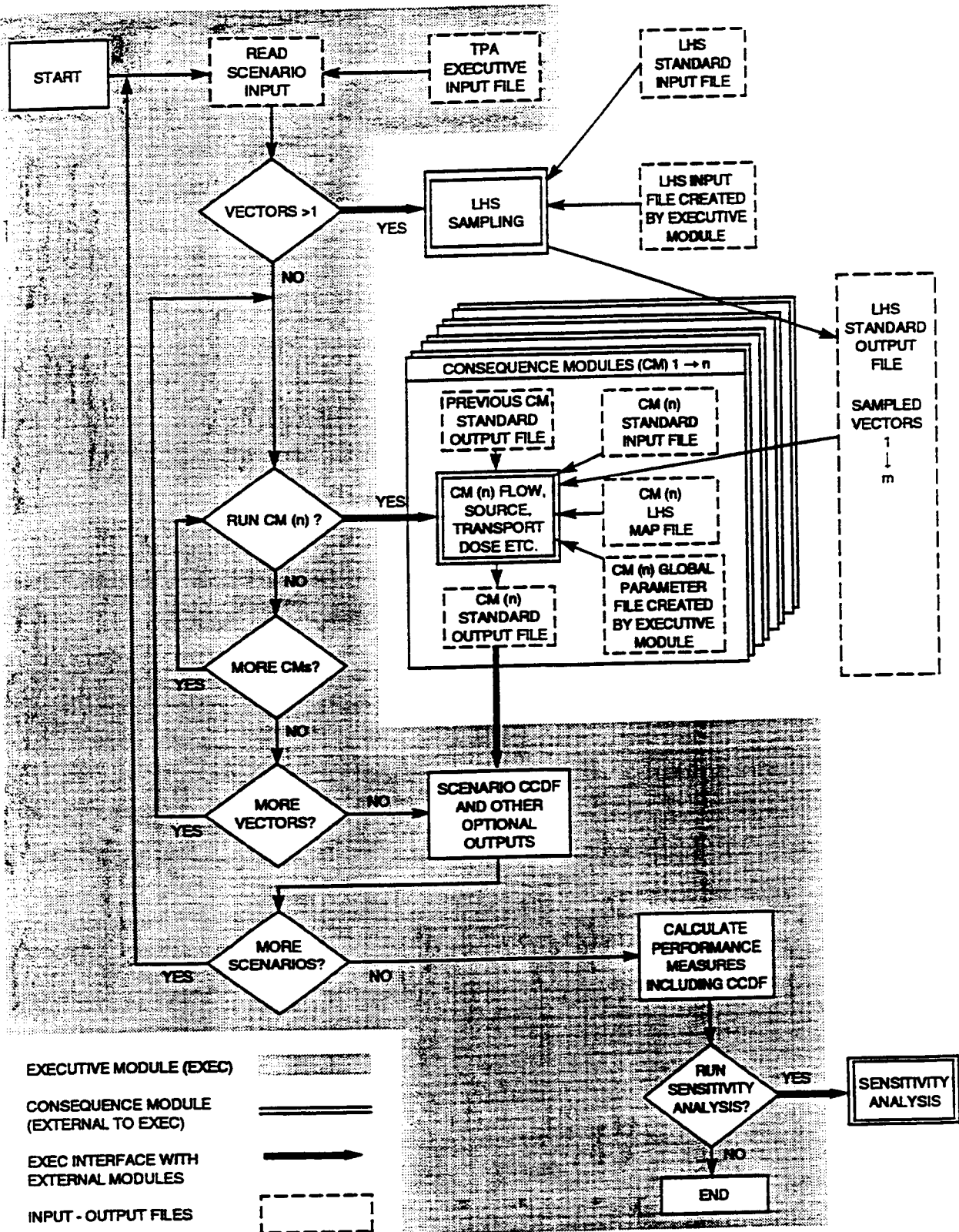


Figure 1-2. Organization of the TPA computer code

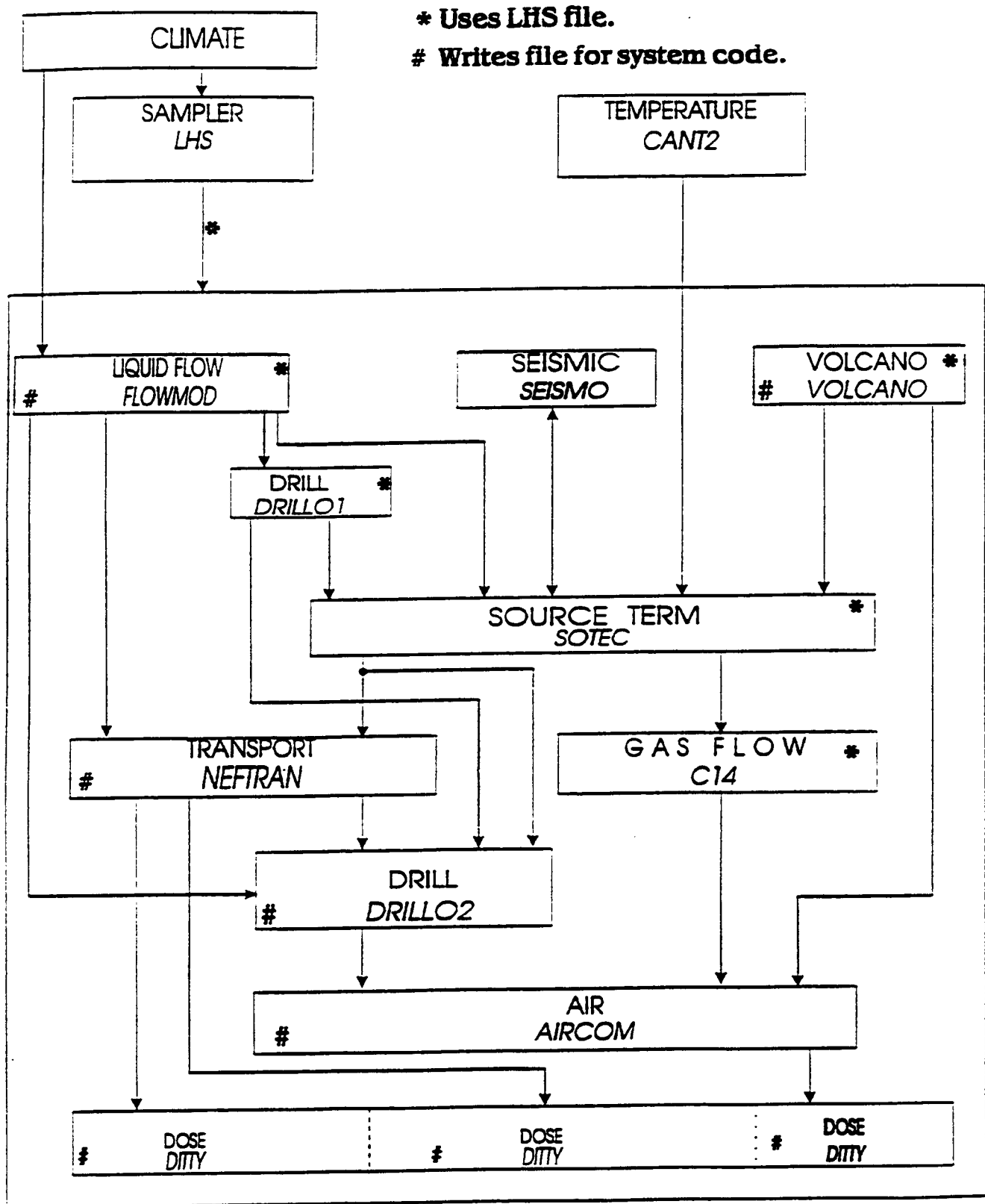


Figure 1-3. TPA system flow diagram

In SEISMO, the strength of the waste packages is influenced by the amount of corrosion (thereby reducing the structural strength of the waste package materials), and therefore, highly-corroded packages are susceptible to failure at lower earthquake magnitudes. Currently, two modes of failure are modeled: (i) base failure; and (ii) impingement failure. SEISMO determines the time at which the waste package fails by comparing the probability associated with the acceleration needed for failure to the probability that there will be an earthquake of that magnitude within the next 10,000 yr. In the event of premature failure of the waste packages in the repository region, these data are then communicated to other modules of the TPA code to allow for transport of the HLW from the repository region.

1.4 REPORT CONTENT

A brief description of the conceptual and mathematical models embodied in the SEISMO code is presented in Chapter 2. Here, the assumptions made in and limitations of the model are presented. Features of the software are described in Chapter 3, which includes a detailed description of the code's capabilities and structure. Chapter 4 contains the input instructions for the SEISMO code. Chapter 5 describes the output from the SEISMO code. The verification and validation status are discussed in Chapter 6. Chapter 7 gives the references. Sample problems are given in the text of the report. Error messages for the SEISMO code are listed in Appendix A.

2 MODEL DESCRIPTION

2.1 OVERVIEW

The SEISMO computer code is designed to model the effects of seismic events on the performance of the potential repository in YM. The code considers the scenario of the release of radionuclides to the geologic media due to seismic events that violate the integrity of the waste canisters in the repository.

YM is located in a region where a number of earthquakes have occurred in the recent past due to extensional faulting which is present in the Basin and Range tectonic province. In addition to large earthquakes, numerous small-scale movements along strike-slip fault zones northwest and southwest of YM have been recorded. This potential for faulting and seismicity at the site of the repository may result in the premature failure of waste packages due to vibratory ground motion (e.g., shaking) or failure due to secondary faulting. Shaking may lead to package failure through: (i) waste package impingement on the borehole wall, (ii) failure of waste package support structure (typically at the base of a package), or (iii) borehole wall failure. A seismic process may also rupture waste canisters through faulting if a canister is inadvertently located in a fault zone. In addition to these direct effects, secondary effects of seismic events may also result in accelerated release and transport of radionuclides. In particular, a seismic event may change regional groundwater flow patterns, lead to short-term elevation changes of the water table, and possibly result in changes to the ground surface infiltration characteristics.

Only two modes of failure are currently modeled in SEISMO Version 1.0: (i) waste package impingement on the borehole wall (impingement failure) and (ii) failure of waste package support structure (base failure). Impingement failure results from a collision of the free-end of the waste canister with the borehole wall, caused by the oscillation of the free-end in response to seismic-generated ground motions. Base failure results from vibration-induced stresses exceeding the yield strength of the waste package at its base, which is assumed to be rigidly attached to the bottom of the borehole. It should be noted that in the design discussed in the Site Characterization Plan (SCP) (U.S. Department of Energy, 1988), the base of the waste package is not anchored to the floor of the borehole. The assumption of rigid attachment can lead to conservative assessment of performance. However, it is not possible to estimate the degree of conservatism because the analysis without this assumption is too complicated and was not performed. More recently, after the completion of SEISMO, Version 1.0, the DOE has proposed entirely new designs using massive multipurpose containers emplaced horizontally. Such a design cannot be analyzed with Version 1.0 of SEISMO.

In the SOTEC code, the physical integrity of a waste canister is modeled, for the case of no seismicity, as a pure corrosion process. The waste canister material is depleted by corrosion, causing the wall thickness to fall below a minimum value dictated by the compressive strength of the material, resulting in collapse of the canister under its own weight. The premise in accounting for seismicity in the SEISMO code is that with seismicity, a lesser degree of corrosion can cause waste package failure when augmented by seismic-generated ground motions. This seismic consequence analysis then determines the time of failure for all packages in a repository area, which is less than the failure time due to corrosion-induced collapse. This seismic analysis relies on the SOTEC module (Sagar et al., 1992) of the TPA code for data on the depth of pitting and crevice corrosion. Premature failures of the waste packages are then communicated back to SOTEC from SEISMO to allow for the early release of radionuclides.

The SEISMO code determines the time at which the waste package fails by comparing the probability associated with the acceleration needed for failure to the probability that there will be an earthquake of that magnitude. This analysis determines the time after emplacement that an earthquake would have an acceleration sufficient in magnitude to cause waste package failure due to impingement or base failure. It is assumed here that if either failure criterion is satisfied, then immediate failure occurs for all canisters in a repository region. The details of this analysis process and its mathematical models are presented in Section 2.2 through 2.4 of this report.

We would like to stress that this is only an initial effort at including seismicity affects in calculating the performance of the total system. The model encoded in SEISMO, Version 1.0 uses seismic hazard curves for a site to estimate possible damage to waste packages emplaced vertically in boreholes. If the DOE elects to change this design (e.g., use of multipurpose canisters emplaced horizontally), then this model will have to be modified significantly.

2.2 RESPONSE OF WASTE PACKAGE TO SEISMIC-GENERATED GROUND MOTIONS

The magnitude of the response of the waste package to seismic-generated ground motions is determined by the maximum displacement of the waste package with respect to the ground or emplacement hole. Here, the waste package is considered to be a hollow, slender, elastic cylinder of length L (unit=m), standing vertically, and attached at the bottom to the ground. Figure 2-1 displays this condition of the waste package being modeled as a vertical, cantilever beam, fixed at the bottom. Several parameters must be accounted for in the calculation of the maximum displacement of the waste package. First, the moment of inertia of the waste package cylinder, I , is given by:

$$I = \frac{\pi}{4} [R^4 - (R - d)^4] \approx \pi R^3 d \quad (2-1)$$

where R is radius of the cylindrical waste package (unit=m), and d is thickness of the cylinder wall (unit=m).

The spring constant K for the waste package is then given by:

$$K = 3EI/L^3 \quad (2-2)$$

where E is the modulus of elasticity of the waste package material (unit= N/m^2).

The total mass of the waste package itself and its contents is required in order to compute the natural frequency of the waste package system. It is assumed that the cylinder is thin walled; therefore, the volume of metal in the top or bottom ends of the cylindrical waste package, V_e , is given by the expression:

$$V_e = \pi R^2 d \quad (2-3)$$

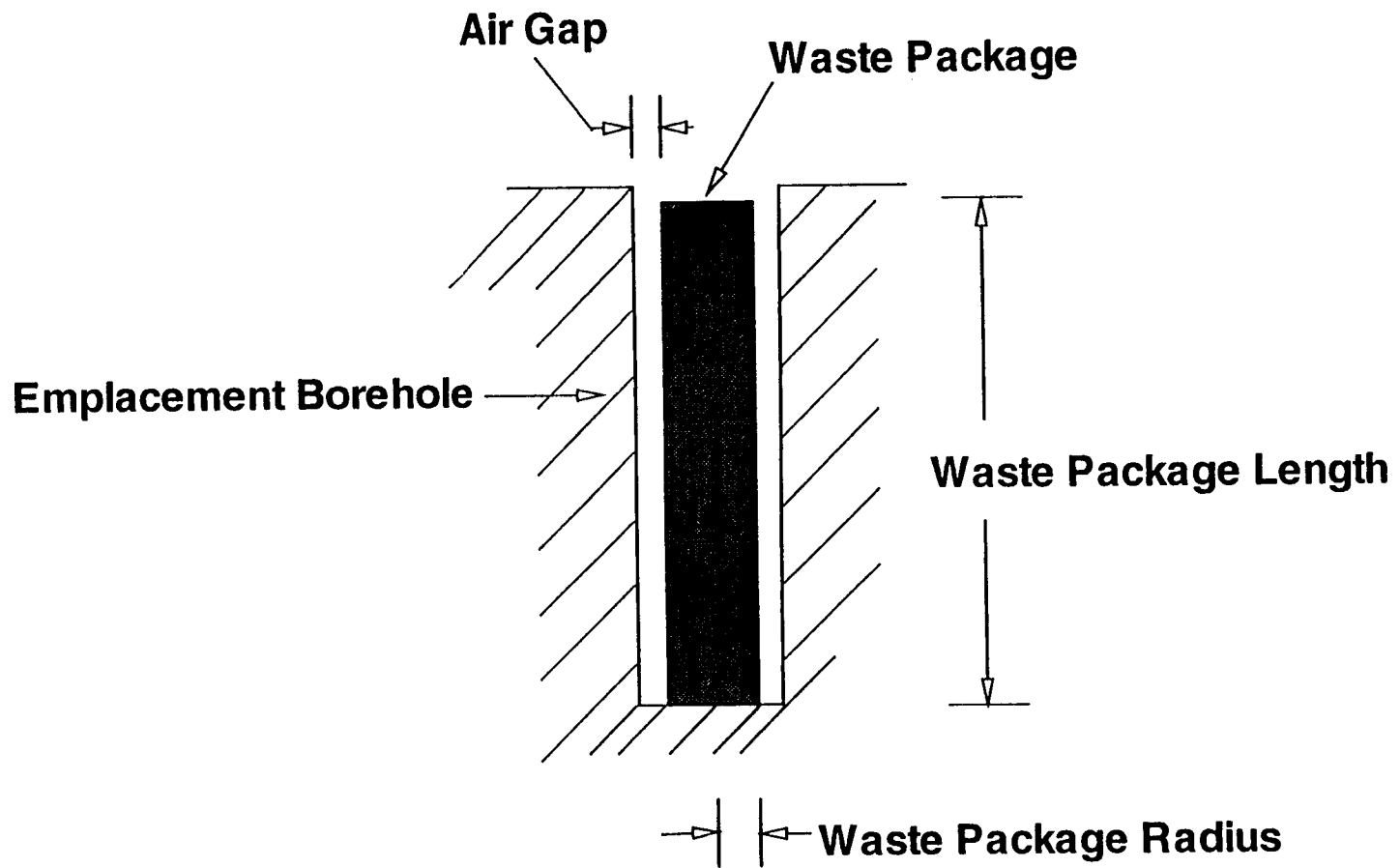


Figure 2-1. Description of waste package modeled as a cantilever beam

and the volume of the cylindrical side, V_s , is given by:

$$V_s = \pi [R^2 - (R - d)^2]L \quad (2-4)$$

and the total volume, V_T , is then given by:

$$V_T = 2V_e + V_s \quad (2-5)$$

Using Eq. (2-5), the mass of the waste package itself is given by:

$$M_p = V_T \rho_{ss} \quad (2-6)$$

where ρ_{ss} is the density of stainless steel (unit= kg/m^3).

The total mass of the waste package system, M_T , is then the sum of the waste package mass, M_p , and the mass of the waste per package, M_w . The mass of the radioactive waste per package, M_w , (unit= Kg) is an input to the code.

The natural or resonant frequency of the undamped, waste package system is given by:

$$\omega_n = \left(\frac{2K}{M_T} \right)^{1/2} \quad (2-7)$$

This equation assumes that half of the total mass of the waste package was located at the top end of the cantilever and half at the bottom end. The mass associated with the base of the waste package is assumed to move with the ground, and thereby, it does not enter into the calculation of natural frequency.

If ω_a is defined as the excitation frequency (unit= Hz), that is the vibrational frequency of the ground motion created by the seismic event, then the ratio of the excitation frequency to the resonant frequency is:

$$\Omega = \omega_a / \omega_n \quad (2-8)$$

For the nominal waste package parameters, the natural or resonant frequency of the waste package system will initially be much higher than that of the excitation frequency, but, as the metal thickness is reduced by corrosion processes, the resonant frequency also decreases. It is then assumed in this analysis that the resonant frequency of the waste package system will never be less than that of the excitation frequency; that is, $\Omega \geq 1$. This adds an additional degree of conservatism to this analysis.

In order to calculate the displacement of the center of mass of the waste package system, denoted by $x(t)$, the motion of the ground is defined by $x_g(t)$ and the relative motion of the mass of the waste package system with respect to the ground (and the emplacement hole) by $x_r(t)$. Then:

$$x_r(t) = x(t) - x_g(t) \quad (2-9)$$

Further, because we are only interested in the steady-state solution (or harmonic solution), then displacement functions may be written in the form:

$$x_g(t) = A_g \sin(\omega_a t) \quad (2-10)$$

$$x_r(t) = A_r \sin(\omega_a t - \phi) \quad (2-11)$$

where A_g and A_r are amplitudes of the ground and waste package displacement, respectively, and ϕ is the phase difference between the ground motion and the waste package movement. Then, for a simple spring-mass system, with damping associated with the velocity term, the ratio of the amplitudes may be written as:

$$\frac{A_r}{A_g} = \Omega^2 / [(1 - \Omega^2)^2 + (2\xi\Omega)^2]^{0.5} \quad (2-12)$$

where ξ is the damping factor.

What remains is to cast Eq. (2-12) into a form that allows the calculation of A_r as a function of frequencies and accelerations only. Because we are assuming a sinusoidal motion, we can easily formulate an equation for ground acceleration by differentiating Eq. (2-10) twice:

$$\ddot{x}_g(t) = -\omega_a^2 x_g(t) = -\omega_a^2 A_g \sin(\omega_a t) \quad (2-13)$$

Further, based on Eq. (2-13), the peak ground acceleration a may be defined to be equal to the amplitude of the acceleration of the ground due to the seismic wave as expressed in Eq. (2-13):

$$a = \omega_a^2 A_g \quad (2-14)$$

Then, the maximum displacement of the waste package system A_r as a function of peak ground acceleration a , excitation frequency ω_a , and the ratio of excitation to resonant frequencies is:

$$A_r = \frac{a\Omega^2}{\left\{ \omega_a^2 [(1 - \Omega^2)^2 + (2\xi\Omega)^2]^{0.5} \right\}} \quad (2-15)$$

This is the amplitude of the waste package system response, which is used to determine failure of the waste packages in a repository region.

2.3 WASTE PACKAGE FAILURE MODES

Two modes of failure are modeled in SEISMO, that is, base failure and impingement failure. Failure Mode 1, base failure, occurs due to seismic-induced, vibrational stresses exceeding the yield strength of the waste package at its base. Specifically, the waste package is assumed to fail if the stress at the base of the waste canister exceeds the yield strength of the waste package material. Failure Mode 2, impingement failure, occurs due to seismic-induced oscillations of the free end of the waste package which swing far enough to impact the side of the emplacement borehole. Specifically, the waste package is assumed to fail if the motion induced at the free end of the waste package is so great that it impinges on the side of the emplacement borehole, causing the waste canister to buckle.

2.3.1 Failure Mode 1—Base Failure

As has been described, Failure Mode 1 is induced when the magnitude of vibration of the waste canister becomes so great that the stress at the base of the canister exceeds the yield strength of the canister material. It is assumed that the waste package is a vertical cantilever beam, fixed at its base to the moving ground plane, and free to move at its top. Under these conditions, stresses will be the greatest at the base of the waste package. The waste package system may then be represented mathematically as a spring-mass system for which the force loads at the base of the canister are considered. The force, F_M , exerted by the movement of the mass at the free end of the cantilever beam can be derived from the definition of the spring constant:

$$F_M = -Kx_r \quad (2-16)$$

where x_r is the deflection of the free end of the waste package. Then, by using the equation for the spring constant [Eq. (2-2)], the moment, M_a , at the base induced by the force, F_M , is given by (Perry, 1967, p. 6-52):

$$M_a = LF_M = -3EIx_r/L^2 \quad (2-17)$$

and the stress at the base of the canister resulting from the moment, M_a , is directly given by:

$$\sigma_a = M_a L/I = -3Ex_r/L \quad (2-18)$$

However, it is the maximum stress induced by the deflection of the free end that is of interest, therefore, the maximum deflection, so x_r can be replaced with A_r , and obtained for the maximum stress at the canister base:

$$\sigma_a = 3EA_r/L \quad (2-19)$$

The failure criterion is then defined as: failure will occur if $\sigma_a \geq \sigma_Y$, where σ_Y is the stress magnitude at the canister material's yield point. This criterion may be restated by:

$$A_r \geq A_{rY} = L\sigma_Y/3E \quad (2-20)$$

2.3.2 Failure Mode 2—Impingement Failure

Failure Mode 2 is induced when the oscillatory motion of the free end of the waste package is so great that it collides with the side of the emplacement borehole, causing the waste canister to buckle. For failure to occur by this mechanism, two conditions must be satisfied:

- (i) The displacement from equilibrium of the free end of the waste package must be large enough so that the package comes in direct contact with the side of the emplacement borehole
- (ii) The force created by the impact of the canister with the emplacement wall must be great enough to buckle the side of the waste package

To determine if condition (i) is satisfied, the amplitude of displacement of the free end of the waste package, given by Eq. (2-15) can be compared to the magnitude of the air gap, W_{ag} defined to be the normal separation distance between the canister side wall and the emplacement borehole side wall. The term W_{ag} is an input parameter to SEISMO, with the current design specifying the value of this parameter to be 1.5 in (3.81 cm) of air gap all around the canister. Condition (i) is then quantified as:

$$A_r \geq W_{ag} \quad (2-21)$$

Condition (ii) is specified in Iterative Performance Assessment (IPA) Phase 2 version of the model by assuming that any contact of the waste package with the side of the borehole emplacement will result in failure. Thus, if condition (i) is satisfied, that is, Eq. (2-21), then condition (ii) is also satisfied, and failure occurs.

It is possible that a waste package that is not attached rigidly to the floor of the borehole as assumed here may slide and impinge on the borehole wall at a lower acceleration. However, we assumed that due to substantial mass of the waste package, the tipping of the waste package about its base was more probable. Of course, the dynamics of the waste package in the nonanchored core will be quite complex which may result in other types of stresses and failure mechanisms.

2.4 COMPUTATIONAL ALGORITHM FOR SEISMIC FAILURE OF WASTE PACKAGES

The prediction of failure of the waste canisters is a time-dependent process. At each time step in the calculation, data on the corroded wall thickness of the waste canister are used. These time-dependent data are supplied by the SOTEC module of the TPA code. These data are calculated from a corrosion model (accounting for general corrosion, plus pitting and crevice corrosion), and do not represent the thickness of the metal as a whole. In this respect, the model is conservative, because the thickness of the remaining metal will be much greater than that in the pits.

In addition to the time-varying values of wall material thickness, several other key parameters are used in SEISMO. All these parameters and their current values are displayed in Table 2-1. Note that

the values in the fourth column are provided as input and not hard coded. Other values may be specified in the input files (see Section 4).

Table 2-1. Parameter definitions used in the SEISMO code

Variable Name	Symbol	Description	IPA Phase 2 Value
<i>PacLeng</i>	<i>L</i>	Package length	4.7625 m
<i>PacRad</i>	<i>R</i>	Package radius	0.3302 m
<i>PacThik</i>	<i>d</i>	Package wall thickness	0.010 m
<i>DampFac</i>	ξ	Damping factor	0.03
<i>ElasMod</i>	<i>E</i>	Modulus of elasticity of package material	$2.0 \times 10^{11} \text{ N/m}^2$
<i>Densss</i>	r_{ss}	Density of stainless steel	$7.75 \times 10^3 \text{ kg/m}^3$
<i>Wmass</i>	M_w	Mass of waste per package	$6.4 \times 10^3 \text{ kg}$
<i>FreqAcc</i>	ω_a	Seismic wave frequency	5 Hz
<i>Ystrg</i>	σ_Y	Package material yield strength	$2.07 \times 10^8 \text{ N/m}^2$
<i>Widthag</i>	w_{ag}	Width of air gap	0.0381 m

Given these data, the critical displacement of the waste package, A_{rc} , is calculated for Failure Mode 1 [Eqs. (2-15) or (2-20)] and Failure Mode 2 [Eq. (2-21)]. The smaller of these two amplitudes is then defined as A_{rc} and is used to determine at what acceleration level the waste package will fail.

To perform this operation, the failure acceleration, a_f , is defined. Although the quantity is not fragility, which is formally defined to be a probability function, it does embody the direct effects of representing the potential for the line. Thus, a_f , which is to correspond to the ground acceleration in g 's resulting from the application of A_{rc} :

$$a_f = A_{rc} \omega_a^2 \left[(1 - \Omega^2)^2 + (2\xi\Omega)^2 \right]^{0.5} / 9.81 \Omega^2 \quad (2-22)$$

The failure acceleration then has a corresponding annual rate of recurrence, r_a , associated with it, which is derived from a curve fit to a published set of data for YM (Blume and Associates, 1987); although these data are limited to 1g, we have assumed the curves fit to apply to 4g. This annual rate of exceedance, r_a , is represented here as:

for $a_f < 0.1 g$

$$r_a = 0.01 \quad (2-23a)$$

for $0.1 g < a_f < 4 g$

$$\log_{10} (r_a) = a_0 + a_1 l + a_2 l^2 + a_3 l^3 + a_4 l^4 + a_5 l^5 + a_6 l^6 \quad (2-23b)$$

for $a_f > 4 g$

$$r_a = 0.0 \quad (2-23c)$$

where:

$$\begin{aligned} l &= \log_{10} (a_f) \\ a_0 &= -4.67174 \\ a_1 &= -4.16482 \\ a_2 &= 1.91376 \\ a_3 &= 3.75132 \\ a_4 &= -3.06375 \\ a_5 &= -2.04791 \\ a_6 &= 1.65667 \end{aligned}$$

Note that the published data of Blume and Associates applies to $a_f \leq 1g$. Thus, Eq. (2-23b) represents an extrapolation of published data and may not be entirely accurate.

The probability that failure of the waste package occurs within the time step t to $t + \Delta t$ is calculated from the annual rate of recurrence, r_a :

$$p\Delta t = 1 - (1 - r_a)^{\Delta t} \quad (2-24)$$

where Δt is measured in number of years for the time step. This equation approximates the Poisson distribution for small values of r_a .

Whether or not failure occurs during a particular time step is a matter of chance. In this model, the failure probability, $p\Delta t$, is compared to a number, U , with magnitude varying between zero and unity, selected randomly from a uniform distribution. If the random number is less than the failure probability, then the waste package is assumed to fail. The random number, U , is sampled once per Latin Hypercube Sampling (LHS) vector, from the main sampling routine of the TPA code, in order to keep all randomness under the control of the system-level program. While it would appear that the random number U should be sampled at each time step within an LHS vector, numerical experiments with the model indicate that the results are essentially the same, statistically, for either case, given a sufficiently large number of vectors.

3 SEISMO SOFTWARE DESCRIPTION

3.1 SOFTWARE CAPABILITIES AND SALIENT FEATURES

The SEISMO computer code calculates a failure time for the waste packages within a given repository region caused by seismic accelerations. It is assumed that all waste packages within a given repository region respond identically, so that only one failure time is calculated per repository region, and all canisters fail at this time within that region.

SEISMO is run as part of the TPA code, and, as such, it interacts with two modules of the TPA code; that is, the TPA Exec module and the SOTEC module. Figure 3-1 displays schematically these interactions between SEISMO and the TPA code modules. From the TPA Exec module, SEISMO receives information on the data file names for input from SOTEC and output to SOTEC. This input file from SOTEC contains time history data of waste package thickness per repository region. The output file, sending data to SOTEC, contains, for each region of the repository, the time of waste package failure (if failure has occurred). Other data received from the TPA Exec are the current vector number (*Vnum*), the duration of simulated time (*StpT*), the length of all waste packages (*PacLeng*), the radius of all waste packages (*PacRad*), the original wall thickness of all waste packages (*PacThik*), the total number of waste packages in the entire repository (*TotCan*), and the total amount of nuclear waste in the entire repository, measured in thousands of metric tons (*waste*). Complete details of this SEISMO Global Data Temporary Input File, *TPA_SEI.SGD*, are given in Sagar and Janetzke (1993).

3.2 SOFTWARE LIMITATIONS

The SEISMO code has no specific computational limitations. The code is currently executable on CRAY, VAX, and Silicon Graphics machines. The source code is written in standard FORTRAN 77 syntax. It is assumed, however, that the existence of various input files (schematically shown in Figure 3-1 and discussed in Section 4) are verified by the analyst prior to execution of the SEISMO module.

3.3 HARDWARE REQUIREMENTS AND INSTALLATION PROCEDURES

The SEISMO computer code requires minimal hardware resources. The largest arrays are dictated by the product of the number of repository regions and the number of time history points for wall thickness data (generated by SOTEC). There are only two arrays of this size, one for the time values and the other for the wall thickness values. Execution time ranges from minutes on VAXes to seconds on CRAYs, and the disk files created by SEISMO are only a few kilobytes in size.

The primary source files are maintained as FORTRAN preprocessor input files. The preprocessor is called preFOR and is discussed in Section 3.4.1 of Sagar and Janetzke (1993). Once the preFOR files are copied to disk, an operating procedure may be written to automatically generate the executable files.

3.4 USER SUPPORT

For technical assistance, the user may contact either:

3-2

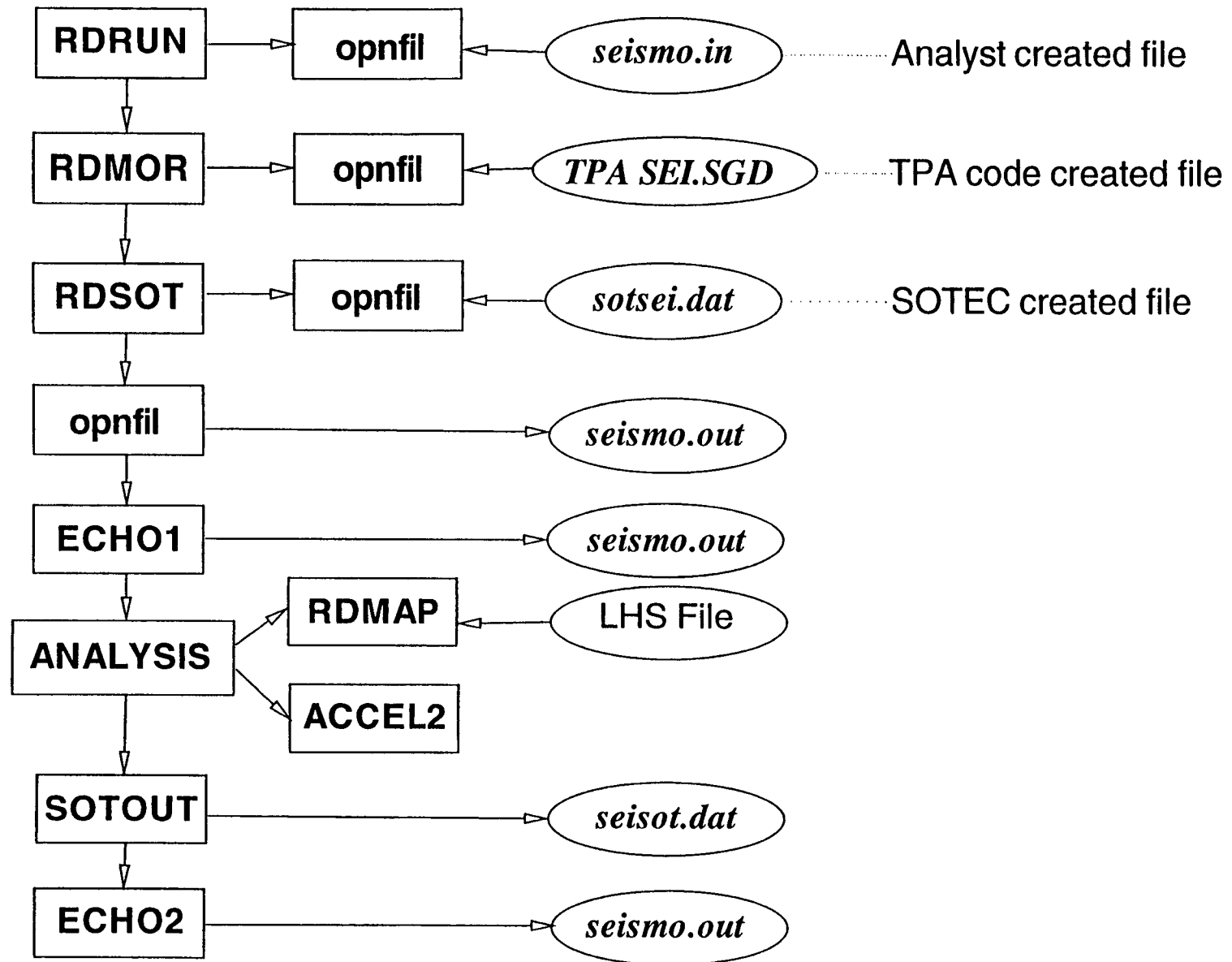


Figure 3-1. Call sequence and input files for SEISMO

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3.5 CODE STRUCTURE

This section describes the purpose and details of each subroutine in SEISMO. Again, the SEISMO computer code calculates a failure time for the waste packages within a given repository region caused by seismic accelerations. Figure 3-1 displays the calling sequence of the subroutines that make up the SEISMO code.

3.5.1 Subroutine RDRUN

Subroutine RDRUN reads input data from the file *seismo.in*, which is an analyst-created file. Input parameters read from *seismo.in* are the duration of the simulation, the radius of the waste canisters, the length of the waste canisters, the initial wall thickness of the canisters, the canister material's modulus of elasticity, the density of the canister material, the mass of nuclear waste per canister, the width of the air gap surrounding the canisters, the damping factor, the critical probability, and the seismic wave frequency.

3.5.2 Subroutine RDMOR

Subroutine RDMOR reads the SEISMO Global Data Temporary Input File, *TPA_SEI.SGD*, if it exists. If *TPA_SEI.SGD* does exist, then several additional data parameters are read in. These are the name of the data file created by SOTEC (containing time history data of wall thickness in each repository region), the name of the data file to be created by SEISMO for input to SOTEC, the vector number of this simulation, the duration of the simulation, the waste package length, the waste package radius, the initial wall thickness of the waste packages, the total number of waste packages in the entire repository, and the total amount of nuclear waste in the entire repository.

If the file *TPA_SEI.SGD* does not exist, then the SEISMO input file name of SOTEC data is specified as *sotsei.dat*, and the SEISMO output file name for SOTEC input is specified as *seisot.dat*.

3.5.3 Subroutine RDSOT

Subroutine RDSOT reads the data file created by SOTEC containing the time histories of waste package wall thickness for each region of the repository. This SOTEC-created file contains multiple vectors of this data, therefore, in subroutine RDSOT, the entire file is scanned until the current vector number, designated by the parameter *Vnum*, is found and then the data are read.

3.5.4 Subroutine ECHO1

Subroutine ECHO1 prints to a file all the initial input parameters and the wall thickness time history data. This diagnostic file is named *seismo.out*.

3.5.5 Subroutine ANALYSIS

Subroutine ANALYSIS directs and performs the primary computations required to predict time of failure of waste packages within a given repository region. The subroutine cycles through each time node of the wall thickness data set, calculating the probability of failure and then determining whether failure has occurred. Specifically, for each data point of wall thickness, subroutine ANALYSIS first determines whether the wall thickness is less than a critical value below which the canister cannot support its own weight. This is currently set at a minimum wall thickness value of 1.0×10^{-10} m. If the current value of the wall thickness is less than this minimum value, then failure has occurred and the time of failure for this repository region is then logged and the next repository region is analyzed. If failure has not occurred, then the moment of inertia, spring constant, and volume of the canister are calculated, as well as the mass and natural frequency of the package and waste. If the seismic wave frequency is longer than the calculated natural frequency of the waste package system, then the seismic wave frequency is set equal to the package's natural frequency, resulting in the ratio of frequencies of unity. Next, the critical failure mode displacement (i.e., the smaller value of the two modes of failure) is determined and the resulting acceleration magnitude calculated. From this, the annual rate of exceedance of an earthquake is calculated, which then allows for the calculation of the probability of failure. If a random number is less than this probability of failure, then failure has occurred, and again, the time is logged, and the cycle begins for the next repository region. If the random number is greater than the probability of failure, then the next time step is selected, and the process repeats for the same repository region.

3.5.6 Subroutine SOTOUT

Subroutine SOTOUT writes data to the file that is used as input to the SOTEC module. Data included in this file are the total number of repository regions, and then for each region, the failure indicator parameter (which means that if it has a value of 1, the canisters have failed; or if it has a value of 0, the canisters have not failed and are maintaining their integrity) and the time of failure (if the canisters have not failed, then the value of time is set to the value of *StpT*).

3.5.7 Subroutine ECHO2

Subroutine ECHO2 writes additional data to the output file *seismo.out*. These additional data are, for each region of the repository, the failure indicator parameter, the time of failure of the waste packages, and the displacement amplitude used to determine failure.

3.5.8 Subroutine ACCEL2

Subroutine ACCEL2 calculates the annual rate of recurrence, a_y , given the fragility, f , and using the discrete distribution defined by Eq. (2-23).

3.5.9 Subroutine RDMAP

Subroutine RDMAP reads the uniform random number, U , from the LHS file. The location of U in the LHS file is currently set as the 444th number of the data set. Again, the random number U is sampled only once per LHS vector.

3.5.10 Subroutine OPNFIL

Subroutine OPNFIL opens a formatted file on the unit specified with the attributes provided in the argument list. This subroutine first determines the availability of the requested unit and file. If either is already in use, then processing is terminated and control is returned to the calling routine. Otherwise, the desired operation is performed.

3.6 INSTRUCTIONS FOR CODE MAINTENANCE

The program preFOR (Janetzke and Sagar, 1991) is a preprocessor for FORTRAN codes. It is designed to provide flexibility in developing and maintaining FORTRAN codes. Included in preFOR are various utility modules to find the length of strings, fix tabs, perform I/O, etc. When invoked, preFOR prompts the user for an input filename. The input file is a FORTRAN source code in which preFOR commands have been embedded. The program then prompts the user for an output filename. The output file produced by preFOR is a standard FORTRAN file that may be compiled. Details of the preFOR command set and its use are documented in Janetzke and Sagar (1991).

3.7 ARRAY SIZES IN SEISMO

The arrays in SEISMO are of a size dictated by two parameters; namely, the number of repository zones ($maxZon$) and the number of time steps ($maxTnd$) defining the wall thickness time histories. All but two of the code's arrays are single-indexed arrays, based only on $maxZon$. The remaining two arrays have a size defined by the product of $maxZon$ and $maxTnd$.

3.8 UNITS IN SEISMO

All units in SEISMO are metric [i.e., meter (length), kilogram (mass), Newton (force), and Pascal (stress)]. Frequency is defined by Hertz (Hz) and time is expressed in terms of years.

4 INSTRUCTIONS FOR DATA INPUT

As already discussed, SEISMO is run as part of the TPA code. The analyst must create at least one input file, that is, *seismo.in*. Other input data files must also exist for proper operation of SEISMO; however, these additional data files are created by the TPA consequence module SOTEC (i.e., the *sotsei.dat* file) or the TPA code itself (i.e., the Global Data Temporary Input File *TPA_SEI.SGD*).

4.1 INPUT DATA FILES FOR SEISMO

SEISMO uses three required data input files. Those required files are *seismo.in* (an analyst created file), the SOTEC-generated data file of time history data of waste package wall thickness, and the Global Data Temporary Input File *TPA_SEI.SGD*.

4.1.1 Description of the *seismo.in* Input File

The *seismo.in* input data file for SEISMO is created by the analyst. This data file is required for TPA mode operation. It contains the following information:

Line 1:	Simulation title
Line 2:	Simulation duration in years, variable <i>StpT</i>
Line 3:	Radius of waste package in meters, variable <i>PacRad</i>
Line 4:	Length of waste package in meters, variable <i>PacLeng</i>
Line 5:	Initial wall thickness of waste package in meters, variable <i>PacThik</i>
Line 6:	Modulus of elasticity of waste package material in Pascals, variable <i>ElasMod</i>
Line 7:	Density of waste package material in kilograms per cubic meter, variable <i>Densss</i>
Line 8:	Yield strength of waste package material in Pascals, variable <i>Ystrg</i>
Line 9:	Mass of nuclear waster per canister in kilograms, <i>Wmass</i>
Line 10:	Width of air gap surrounding a waste package in meters, variable <i>WidthAG</i>
Line 11:	Damping factor, variable <i>DampFac</i>
Line 12:	Critical Probability, variable <i>ProbAcc</i> (not currently used)
Line 13:	Seismic wave frequency in Hz, variable <i>FreqAcc</i>

Example of the *seismo.in* data file:

```
INPUT FILE TO SEISMO
10000.0      Duration of Simulation (years)
0.3302      Radius of waste canisters (meters)
4.7625      Length of waste canister (meters)
0.010       Thickness of waste canister (meters)
2.00E+11    Modulus of elasticity of waste canister material (N/m2)
7.75E+03    Density of waste canister material—stainless steel (kg/m3)
2.067E+08   Yield strength of canister material (N/m2)
6.40E+03    Mass of waste per waste canister (kg)
0.0381     Width of air gap around waste canister (m)
0.030      Damping factor for a waste canister
0.990      Critical probability (not used)
5.00       Seismic wave frequency (Hz)
```

4.1.2 Description of the *TPA_SEI.SGD* Input file

The input file *TPA_SEI.SGD* is created and maintained by the TPA code. If this data file does not exist, then the SEISMO code will not run properly. Global data read from this file are as follows:

Line 1: Simulation title
Line 2: Input file name of SOTEC data, that is, wall thickness time histories
Line 3: Output file name for SOTEC input data, that is, waste package failure times
Line 4: Current vector number; variable name = *Vnum*
Line 5: Simulation duration in years, variable name = *StpT*
Line 6: Length of waste package in meters, variable *PacLeng*
Line 7: Radius of waste package in meters, variable *PacRad*
Line 8: Initial wall thickness of waste package in meters, variable *PacThik*
Line 9: Total number of waste packages in the entire repository, variable *TotCan*
Line 10: Total mass of waste in the entire repository in thousands of metric tons, variable *waste*

Example of the *TPA_SEI.SGD* data file:

```
GLOBAL PARAMETERS FOR SEISMO
sotsei.dat
seisot.dat
1
10000.0
4.7625
0.3302
0.010
25008
176.6
```

4.1.3 Description of the SOTEC-Generated Input file

The SEISMO computer code requires for execution, time history data of waste package wall thickness. These data are read into SEISMO from a data file created by the SOTEC module of the TPA code. These data consist of time values and corresponding wall thickness values for canisters in each region of the repository. In addition, multiple vectors of time history data may be contained within the file, as illustrated in the example file displayed below.

Example of the SOTEC generated data file:

```
TITLE: Container wall thickness from SOTEC to SEISMO.
1      = vector
7      = number of cells
500    = number of times

Cell Time Thickness
1 20. 0.1000000E-01
2 20. 0.1000000E-01
3 20. 0.1000000E-01
```

4 20. 0.1000000E-01
 5 20. 0.1000000E-01
 6 20. 0.1000000E-01
 7 20. 0.1000000E-01
 1 40. 0.9959999E-02
 2 40. 0.1000000E-01
 3 40. 0.1000000E-01
 4 40. 0.1000000E-01
 5 40. 0.1000000E-01
 6 40. 0.1000000E-01
 7 40. 0.1000000E-01

 1 4400. 0.1240006E-02
 2 4400. 0.3320009E-02
 3 4400. 0.2760011E-02
 4 4400. 0.2120012E-02
 5 4400. 0.2880010E-02
 6 4400. 0.3880006E-02
 7 4400. 0.2480012E-02

 1 10000. 0.0000000E+00
 2 10000. 0.0000000E+00
 3 10000. 0.0000000E+00
 4 10000. 0.0000000E+00
 5 10000. 0.0000000E+00
 6 10000. 0.0000000E+00
 7 10000. 0.0000000E+00

TITLE: Container wall thickness from SOTEC to SEISMO.

2 = vector
 7 = number of cells
 500 = number of times

Cell	Time	Thickness
1	20.	0.1000000E-01
2	20.	0.1000000E-01
3	20.	0.1000000E-01
4	20.	0.1000000E-01
5	20.	0.1000000E-01
6	20.	0.1000000E-01
7	20.	0.1000000E-01
1	40.	0.9959999E-02
2	40.	0.1000000E-01
3	40.	0.1000000E-01
4	40.	0.1000000E-01
5	40.	0.1000000E-01
6	40.	0.1000000E-01
7	40.	0.1000000E-01

 1 4400. 0.1240006E-02
 2 4400. 0.3320009E-02
 3 4400. 0.2760011E-02
 4 4400. 0.2120012E-02


```
5 4400. 0.2880010E-02
6 4400. 0.3880006E-02
7 4400. 0.2480012E-02
-----
1 10000. 0.0000000E+00
2 10000. 0.0000000E+00
3 10000. 0.0000000E+00
4 10000. 0.0000000E+00
5 10000. 0.0000000E+00
6 10000. 0.0000000E+00
7 10000. 0.0000000E+00
```

4.1.4 Description of the LHS Input file

An LHS input file is required for the proper execution of SEISMO. The value of the 444th data entry in this file is used by SEISMO to define the uniform random number, U , that is used in the analysis. A complete description of the LHS input file is given in Sagar and Janetzke (1993).

5 DESCRIPTION OF OUTPUT FILES

SEISMO creates two types of output files, one for user diagnostics and information and one for input to the SOTEC module of the TPA code. The user diagnostics and information file is named *seismo.out*. The SOTEC input file created by SEISMO may have an arbitrary name, but one that is defined in the *TPA_SEI.SGD* file.

5.1 USER DIAGNOSTICS AND INFORMATION OUTPUT FILE

As discussed above, SEISMO creates one user diagnostics and information file, that is, *seismo.out*. This file contains the user- and TPA-defined input data and the results from the analysis.

Example of the output file *seismo.out*:

ECHO OUTPUT FROM SEISMO PROGRAM

```

          T : TPA Mode?
sotsei.dat : DATA FILE, OUTPUT FROM SOTEC RUN
sotsei.dat : DATA FILE, INPUT FOR SOTEC RUN

1          : Vector Number
10000.00   : Simulation Stop Time - years
0.330200E+00 : Radius of waste canister - m
0.476250E+01 : Length of waste canister - m
0.100000E-01 : Initial Thickness of waste canister - m
0.200000E+12 : Modulus of Elasticity for canister - N/m2
0.206700E+09 : Yield Strength of canister material - N/m2
0.775000E+04 : Density of canister material - Kg/m3
0.640000E+04 : Mass of waste per canister - Kg
0.381000E-01 : Air Gap width - m
0.0300     : Canister damping factor
0.9900     : Critical probability
5.0000     : Seismic wave frequency

7          : Number of repository zones
500        : Number of time nodes in SOTEC data
```

zone #	time	thickness
1	20.00	0.100000E-01
1	40.00	0.996000E-02
1	60.00	0.992000E-02
1	80.00	0.988000E-02
1	100.00	0.984000E-02
-	-----	-----
1	9900.00	0.000000E+00
1	9920.00	0.000000E+00
1	9940.00	0.000000E+00
1	9960.00	0.000000E+00

1	9980.00	0.000000E+00
1	10000.00	0.000000E+00
zone #	time	thickness
2	20.00	0.100000E-01
2	40.00	0.100000E-01
2	60.00	0.100000E-01
2	80.00	0.100000E-01
2	100.00	0.100000E-01
-	-----	-----
2	9900.00	0.000000E+00
2	9920.00	0.000000E+00
2	9940.00	0.000000E+00
2	9960.00	0.000000E+00
2	9980.00	0.000000E+00
2	10000.00	0.000000E+00

zone #	time	thickness
3	20.00	0.100000E-01
3	40.00	0.100000E-01
3	60.00	0.100000E-01
3	80.00	0.100000E-01
3	100.00	0.100000E-01
-	-----	-----
3	9900.00	0.000000E+00
3	9920.00	0.000000E+00
3	9940.00	0.000000E+00
3	9960.00	0.000000E+00
3	9980.00	0.000000E+00
3	10000.00	0.000000E+00

zone #	time	thickness
4	20.00	0.100000E-01
4	40.00	0.100000E-01
4	60.00	0.100000E-01
4	80.00	0.100000E-01
4	100.00	0.100000E-01
-	-----	-----
4	9900.00	0.000000E+00
4	9920.00	0.000000E+00
4	9940.00	0.000000E+00
4	9960.00	0.000000E+00
4	9980.00	0.000000E+00
4	10000.00	0.000000E+00

zone #	time	thickness
5	20.00	0.100000E-01
5	40.00	0.100000E-01
5	60.00	0.100000E-01
5	80.00	0.100000E-01
5	100.00	0.100000E-01
-	-----	-----
5	9900.00	0.000000E+00
5	9920.00	0.000000E+00
5	9940.00	0.000000E+00
5	9960.00	0.000000E+00
5	9980.00	0.000000E+00
5	10000.00	0.000000E+00

zone #	time	thickness
6	20.00	0.100000E-01
6	40.00	0.100000E-01
6	60.00	0.100000E-01
6	80.00	0.100000E-01
6	100.00	0.100000E-01
-	-----	-----
6	9900.00	0.000000E+00
6	9920.00	0.000000E+00
6	9940.00	0.000000E+00
6	9960.00	0.000000E+00
6	9980.00	0.000000E+00
6	10000.00	0.000000E+00

zone #	time	thickness
7	20.00	0.100000E-01
7	40.00	0.100000E-01
7	60.00	0.100000E-01
7	80.00	0.100000E-01
7	100.00	0.100000E-01
-	-----	-----
7	9900.00	0.000000E+00
7	9920.00	0.000000E+00
7	9940.00	0.000000E+00
7	9960.00	0.000000E+00
7	9980.00	0.000000E+00
7	10000.00	0.000000E+00

TIME OF FAILURE PER ZONE

zone #	failure	time of failure	amplitude	case1
1	1	1160.0000	0.001641	1
2	1	1540.0000	0.001641	1
3	1	1440.0000	0.001641	1
4	1	1320.0000	0.001641	1
5	1	1460.0000	0.001641	1
6	1	1660.0000	0.001641	1
7	1	1380.0000	0.001641	1

5.2 SEISMO-GENERATED OUTPUT FILE FOR SOTEC

As indicated above, SEISMO creates a data output file for the SOTEC module of the TPA code. This file contains time of failure of waste packages in each region of the repository. The output file name is either specified in the *TPA_SEI.SGD* file or is defaulted to *seisot.dat* by the code.

Example of the SOTEC input file:

SEISMO INPUT DATA TO SOTEC

7

zone	failure	time of failure
1	1	1160.0000
2	1	1540.0000
3	1	1440.0000
4	1	1320.0000
5	1	1460.0000
6	1	1660.0000
7	1	1380.0000

6 VERIFICATION, BENCHMARKING, AND VALIDATION STATUS

The SEISMO code was verified through a line-by-line analysis and through a debugging step in which the code was executed line-by-line in a symbolic debugger. The output data were verified for a range of input parameters. The SEISMO code is managed under procedures set out in the CNWRA Technical Operating Procedure (TOP)-018. The production of this user's manual is one of the requirements of TOP-018. No known codes are suitable for benchmarking the SEISMO code. Because of the nature of the process simulated (i.e., a stochastic process occurring over long time periods), validation by comparison to data is also not possible.

7 REFERENCES

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APPENDIX A
ERROR MESSAGES

ERROR MESSAGES FROM SEISMO

SEISMO could not find vector number *Vnum* in file, *SOTEC Input file name*.

SEISMO could not find LHS file, *LHS file name*.

Vector number is different in files TPA_SEI.SGD and, *LHS file name*.

OPEN OPERATION INCOMPLETE. Check opnfil SOURCE CODE.

Unit is open. Use of OPNFIL requires a closed unit.

File is in use, probably on another unit or by another user.

Requested READ file was not found.

NEW file creation blocked by existing file.

File status request is not valid.