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Benchmark Problems **for Waste Package Computer Codes**

Draft Report

Submitted to:

Division of Waste Management Office of Nuclear Materials Safety & Safeguards U.S. Nuclear Regulatory Commission Washington, D.C. 20555 NRC FIN B6985

Submitted by:

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### NUREG/CR-XXXX

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Draft Report

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#### ABSTRACT

This report provides benchmark problems for computer codes that can be used for analysis of a high-level waste package. Problems with analytical solutions, hypothetical waste package design problems, and problems simulating field experiments are presented. Types of problems include heat transfer, stress analysis, radiation shielding, corrosion and leaching, and near-field geochemistry. Specific phenomena addressed include thermal conduction, convection, and radiation; elastic and plastic stress analysis; creep; particle transport for shielding analysis; empirical analysis of corrosion and leaching; and elevated temperature geochemistry.



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### 1.0 **INTRODUCTION 1.1** Background

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The effective management of high-level radioactive wastes is essential to protect public health and safety. The Department of Energy (DOE), through responsibilities inherited from the Energy Research and Development Administration (ERDA) and the Atomic Energy Commission (AEC), and the authority granted in the Nuclear Waste Policy Act, is charged with the safe disposal of these wastes. The Nuclear Regulatory Commission (NRC), through authority granted by the Energy Reorganization Act of 1974, which created the NRC, and the Nuclear Waste Policy Act, is responsible for the regulation of high-level waste management.

The Environmental Protection Agency (EPA) has the authority and responsibility for setting general standards for radiation in the environment. The NRC is responsible for implementing these standards in its licensing actions and for ensuring that public health and safety are protected. The NRC has promulgated technical criteria for regulating the geologic disposal of HLW which incorporate the EPA standard. (The draft EPA standard was published in the Federal Register dated December 29, 1982.) NRC's technical criteria are intended to be compatible with a generally applicable environmental standard. The performance objectives and criteria address the functional elements of geologic disposal of HLW and the analyses required to provide confidence that these functional elements will perform as intended. These technical criteria are described in Chapter 10, Code of Federal Regulations, Part 60 (10 CFR 60).

In discharging its responsibility, the NRC must review DOE repository performance assessments and independently evaluate the performance of the repositories that the DOE seeks to license. Because of the complexity and multiplicity of these performance assessments, computerized simulation modeling is used. Computer simulation models provide a means to evaluate the most important processes that will be active in a repository,

thereby permitting assessment and prediction of repository behavior. Another factor necessitating the use of models is that the time frames associated with high-level waste management range from decades to tens of thousand of years.

Accordingly, the NRC is developing models and computer codes for use in supporting these regulations and in reviewing proposed nuclear waste management systems. Independently, the DOE is also developing models and computer codes for use in assessing repository sites and designs. The analytical model and code development effort must include a procedure for independent evaluation of the tool's capability to simulate real processes. Codes must be evaluated to determine their limitations and the adequacy of supporting empirical relations and laboratory tests used for the assessment of long-term repository performance.

### **1.2** Scope of This Report

This report is one in a series that deals with the independent evaluation of computer codes for analyzing the performance of a high-level radioactive waste repository. The codes used for repository performance assessment have been divided into the following categories: (1) repository siting, (2) radiological assessment, (3) repository design, (4) waste package performance, and (5) overall systems.

Repository siting requires consideration of events at a distance from the repository. Far-field processes include saturated flow, unsaturated flow, surface water flow (flooding routing), solute transport, heat transport, combined solute and heat transport, geochemistry, and geomechanical response.

Radiological assessment includes the development of source terms, the calculation of radionuclide concentrations in the environment, and the -analysis of food pathways, dose-to-man, and expected mortality rates.

Repository design covers areas often called the "near-field." The processes in the repository design area include heat transport, flow in fractured media, and rock mechanics.

The waste package code area deals with the very near-field, primarily the interactions that take place within the waste package and the waste package's interactions with the repository host rock. Included are heat transfer, stress analysis, and chemical interactions such as corrosion.

Overall systems include subcategories of the other categories. For example, overall systems codes may consider aspects of radiological assessment, waste package performance, economic cost (e.g., cost/benefit analysis), repository performance, natural multibarrier performance, or probabilistic aspects of repository performance.

The first step in computer code benchmarking is to select the codes potentially useful for thermal and structural analysis. The next step is to summarize the nature of each selected code and then to prepare benchmark problems for code testing. As a prerequisite to designing benchmark problems, the data that will be used in the problems should be summarized. Thus, three reports will be issued for waste package codes: (1) a model summary report (already prepared), (2) a data set report, and (3) a report describing the benchmark problems to be used in code testing. This report is the benchmark problem report for waste package codes.

### 1.3 Processes Considered

The processes considered in waste package analysis include: heat transfer, engineering mechanics, radiation shielding, corrosion, leaching, and estimation of the waste package geochemical environment. This report provides benchmark problems for each of these areas.

Heat transfer analysis is required to estimate the temperature rise in the initial period of repository operation and during the period following

repository decommissioning. The temperature is important because it must be controlled to allow retrieval of wastes within 50 years, if required. For the longer term performance of the waste package systems, temperatures must be controlled to limit the degradation of or physical and chemical changes to the waste package, canister, and engineered barriers.

Heat transfer phenomena considered include conduction, convection, and radiation. Thermal analysis may include either steady-state or transfer conditions and may be either linear or non-linear. Non-linear analysis may be needed to model materials with temperature-dependent properties such as specific heat or thermal conductivity and heat flow with nonlinear boundary conditions. Results of thermal analyses in the form of temperature distributions may be used as the input to stress analysis codes to estimate thermal-induced stresses.

Engineering mechanics analyses will be required to estimate the stress and deformation of the waste package after emplacement. Stresses and displacements may be caused by hydrostatic and lithostatic pressure, swelling of backfill material, creep, and thermal loading. Dynamic analyses may be required to estimate loads on the waste package and its contents during shipping or in accidents. Both static and dynamic analyses must be considered for linear as well as non-linear material behavior to assess the performance of the waste package during handling, operation, emplacement, and the decommissioning and long-term storage of waste.

Radiation shielding analyses will be required to estimate the radiation field surrounding the waste package during transportation, repository handling operations, and during the post-emplacement phases. During transportation handling, the radiation field around the waste package must be known in order to estimate the potential dose-to-man. Following emplacement of the waste package, radiation shielding analyses are required to estimate the radiation dose to the host rock and any packing material surrounding the waste package. Dose to geologic and packing materials must be considered to determine whether those materials will be

estimation of the waste package geochemical environment. This report provides benchmark problems for each of these areas.

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Radiation shielding analyses will be required to estimate the radiation field surrounding the waste package during transportation, repository handling operations, and during the post-emplacement phases. During transportation handling, the radiation field around the waste package

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degraded by cumulative or instantaneous radiation dose. Radiation dose may also be important in estimating the geochemical environment, especially if the dose rate is high and causes significant radiochemical changes in the very near field surrounding the waste package.

No widely accepted analytical methods exist to estimate corrosion and leaching of waste package canister or waste form materials from first principles. Most of the existing work on waste canister corrosion and waste form leaching is based on the use of experimental data to formulate empirical relationships describing the waste canister and waste form performance over time. The problems presented in this report are designed as verification problems for the code WAPPA proposed by DOE for use in the assessment of overall waste package performance.

Geochemical analysis of the very near-field will be needed to determine the environment in which the waste canister and waste form will perform. The corrosion and leaching behavior of waste package materials is highly dependent on concentrations of chemical species in the very near field. An accurate assessment of chemical speciation will require treatment of elevated temperatures. This generally will require the use of a geochemical analysis code.

### **1.4 Previous Work**

The most extensive testing of codes useful in waste package performance assessment has been done during the development of the individual codes. The documentation available with most codes generally contains from 2 up to as many as 100 problems that have been solved by the code and checked against analytical solutions. These verification problems almost always show excellent agreement with theoretical problems because these are the types of problems used during code development to find "bugs" in the code and to correct the code. In addition, the developers are likely to be more familiar with the code capabilities than are future users and can thus set up a problem consistent with the solution method.

Although most of the routines in a code should have been tested by the developer before the code's release, codes should also be tested by an independent user on a problem or problems developed independently. Studies with this as an objective include the following:

- Westinghouse Electric Corporation Advanced Energy System Division conducted a five-year study of spent fuel dry storage testing at the Engine Maintenance, Assembly, and Disassembly (EMAD) facility on the Nevada Test Site. This project gathered field data on spent fuel temperature profiles in a geometry similar to that which may be encountered in a waste package.
- \* General Electric gathered data on the radiation field surrounding PWR and BWR fuel assemblies in both air and water at its GE Morris facility. These data were used to compare actual measured data with results predicted by QAD-IV.
- An extensive comparison of geochemical codes conducted under the auspices of the American Chemical Society.

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### 1.5 Model Verification and Validation

The testing of waste package performance assessment models can be divided conceptually into two phases, code verification and code validation. As used in this report, code verification refers to testing the performance -of the code. Code validation refers to testing the code against actual physical data obtained from field tests.

Two types of problems can be used for code verification. Problems with known analytical solutions can be used to test the code's numerical solution methods. These will indicate the accuracy of the code and also point out areas where the code may be in error. The second type includes hypothetical waste package problems. These can be used to determine whether the code can simulate interactions likely to occur in a waste package design.

The validation of codes involves gathering data from field tests and comparing the results of the computer model to these field data. The advantage of field validation is that both the code and the mathematical model are tested against the actual physical performance of the waste package concept being modeled. Although this should be an ideal method of testing a code, in reality, this is not the case because several sources of error are possible in the field validation process. These include inaccuracies associated with:

- Inadequate field test data  $\bullet$
- The measurements themselves
- Transcription or transmission of data
- Difficulty in modeling boundary conditions as they occur in the field
- Non-homogeneity of materials
- Approximations necessary for numerical modeling

The code validation process provides an estimate of the ability of an analytical method to predict the overall response of the system and assists in quantifying data inaccuracies in code predictions.

### 1.6 Problem **Specifications**

The problems described in this report fall into three categories: problems for which analytical or semi-analytical solutions are available, hypothetical problems, and problems based on laboratory or field studies. Problems for which analytical or semi-analytical solutions are available provide a direct means for verifying the correctness of formulation and the accuracy of basic segments of a code's solution algorithm.

Since analytical solutions are based on several restrictive assumptions and are limited to simple cases, several realistic problems, some of which correspond to actual field simulations, have been included in the test series to verify segments of numerical codes that may not otherwise be tested. Two modes of evaluation are available for-these problems. First, answers can be compared to simulations using other codes; if major differences in results arise, further investigation is needed. Second, spatial and temporal discretizations can be refined to see if numerical results are convergent. It should be noted that convergence is a necessary but not conclusive indicator of code accuracy.

Besides providing a means of testing a code's solution algorithm, these problems (especially the hypothetical problems and problems based on field or laboratory studies) provide a means of exposing other difficulties that may arise in the practical application of a code. The sources of these other difficulties include inconsistencies between input instructions and the code's actual input requirements, cumbersome input requirements, incompatibilities between codes where output from one code is needed as input to another, and poor output format (for example, too few significant figures).

The description of each problem, in general, consists of the following:

- Problem statement
- Objectives
- Analytical solution, semi-analytical solution, or physical description
- Assumptions
- Input specifications
- Output specifications
- Comments

The problem statement describes the problem and the processes and conditions being considered. The objective section explains what feature of the code the problem will test. If an analytical or semi-analytical solution is available, the solution is described in the next segment. For the hypothetical and validation problems, the physical system being simulated is described. The assumption section specifically lists the assumptions.

The input specifications restate the physical description in terms that can be included in the model. They include values for all necessary physical properties. All required input data must be accurately and completely stated so that results can be reproduced accurately.

Output specifications include the desired solution's specified spatial locations and times. In some cases these results are best presented in graphic form. Comments include any anticipated problems or other information that might be useful to those running the codes.

Grid sizes and time steps have not been specified for problems. This will permit the use of different values for different codes, so as to optimize the use of each code.

The hypothetical problems presented here have not been actually run. Before a problem can be adopted for use as a benchmark problem, it is

important to run it on one or more codes. This is necessary to verify that the problem is well posed and reasonably tractable and to adjust values of input parameters to obtain outputs that will be most sensitive to imperfections in the codes.

### 2.0 THERMAL ANALYSIS CASE PROBLEMS

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This section is primarily concerned with heat transfer by conduction. Heat transfer by convection and radiation are also considered to complete the thermal analysis required for a waste package and to estimate accurately the thermal loads to be used for mechanical analyses. Mathematical model representing these forms of heat transfer consist of differential equations together with appropriate boundary and initial conditions that express conservation of energy and describe the temperature over the region of interest. In the most generalized form, the equations model transient and non-uniform heat transfer with non-linear material properties. The generalized form of the heat transfer equations can be solved analytically or semi-analytically only if simplifications are made.

The literature contains well-established analytical and numerical solutions ranging from the very simple to the complex. For example, in the verification of ANSYS code alone, the developers used over 40 problems ranging in complexity from one-dimensional conduction through a wall to the three-dimensional cooling of a fin (Reference DE-82). Benchmark problems have been selected that represent the code features required for waste package analysis. These features include conduction (linear and non-linear), radiation, convection, and heat transfer in one and two dimensions.

### 2.1 Steady-State Radial Conduction Heat Transfer in a Hollow Cylinder - Temperature Distribution Solution (Similar to problem solved by Kreith, Reference KR-58, pp. 25-27)

Problem Statement. This problem is designed to determine the steady-state radial temperature distribution in a hollow cylinder of inside radius ri and outside r<sub>o</sub> when a region of radius r<sub>W</sub> (r<sub>W</sub> > r<sub>i</sub>) has a known volumetric heat generation rate of q''' that is spatially uniform and the outside surface (r =  $r_0$ ) temperature has a known value of T $_0$ .

A sketch of the geometry is shown in Figure 2.1-1.



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Hollow Cylinder with Steady-State Radial Conduction for Which the Radial Temperature Distribution Will Be Determined

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The thermal conductivity of the material in the annulus is assumed to be constant and independent of temperature.

The differential equation is

$$
\frac{d}{dr} \left( r \frac{dT}{dr} \right) = 0 \tag{1}
$$

in the region  $(r_i \le r < r_0)$ . The boundary conditions are:

$$
at r = r_0 \qquad T = T_0 \tag{2}
$$

at 
$$
r = r_i
$$
  $Q = -k2\pi r_i \frac{dI}{dr} \bigg|_{r = r_i}$  (3)

where

 $T = temperature$   $[\theta]$ \*  $r =$  radial position  $\lceil \ell \rceil$  $r_i$  = inside radius of hollow cylinder [ $\ell$ ]  $r_0$  = outside radius of hollow cylinder [2]  $k =$  thermal conductivity of cylinder material [e/tle]  $\ell$  = length of cylinder  $[\ell]$  $Q =$  heat cylinder flow rate to the hollow on the inside surface  $[e/t]$ inside surface

 $*$  When an equation is presented, the generalized dimensions of the quantities are given in brackets. They are:  $\ell$  = length or distance;  $t = time$ ;  $f = force$ ;  $m = mass$ ;  $\theta = temperature$  change or temperature;  $e =$  energy (which is equal to the product of  $f(x)$ .

The heat flow rate to the hollow cylinder at steady-state is related to the heat generation rate per unit volume within the solid cylindrical region of radius  $r_w$  by

$$
Q = q''' \pi r_w^2 \ell
$$

(4)

where

q " '= volumetric heat generation rate in the heat source region (O < r < r<sub>w</sub>)  $[e/t2^3]$  $r_W$  = outside radius of cylindrical heat generating region [2]

Objectives. The solution to this problem can be used to verify the accuracy of a program's thermal model. This is the heat conduction problem that the WAPPA model (Reference CO-84) solves for each engineered barrier surrounding the waste form.

Analytical Solution. The analytical solution for the temperature distribution in the region  $r_i \le r \le r_0$  is:

$$
T = T_0 + \frac{0}{2\pi k\ell} \quad \ln(\frac{r_0}{r})
$$

(5)

(6)

This solution can also be written in terms of the heat generation rate in the region  $0 \le r \le r_w$  as:

$$
T = T_0 + \frac{q^{1/1}r_W^2}{2} k \ln \frac{r_0}{r}
$$

where  $r_w \leq r_i$ .

Using the last expression, the temperature at the inside surface  $(r = r_i)$ is given by

$$
T_i = T_0 + \frac{q' \cdot r_w^2}{2k} n \frac{r_0}{r_i}
$$

This equation is used successively over the engineered barriers in WAPPA proceeding inward from the outermost annular region.

(7)

#### Assumptions.

- The hollow cylinder material has a unique value for thermal conductivity that is independent of temperature.
- Axial heat conduction is negligible in comparison to radial heat conduction.
- The heat generation is uniform over the cylinder of radius rw.

### Input Specifications.

Geometry (similar to the defense high-level waste cast-iron overpack, Reference ON-83, pp. 33 and 199) waste region radius hollow cylinder inside radius hollow cylinder outside radius  $r_w = 30.5$  cm  $r_i = 30.5$  cm  $r_0$  = 67.5 cm Material properties  $thermal$  conductivity  $k = 0.5$  w/cm<sup>o</sup>C Boundary conditions hollow cylinder outside temperature waste region volumetric heat generation rate  $T_0 = 200^{\circ}C$  $q'''' = 0.001291$  w/cm<sup>3</sup>

Output Specifications. The temperature distribution T(r) in the hollow cylinder  $r_i \le r \le r_0$  is to be determined.

Values at discrete points from  $r_i < r < r_0$  are presented below as determined for the input quantities and Equation 6.



**2.2 Steady-State Radial Conduction Heat Transfer in** a Series of **Concentric Cylindrical Annuli for a Specified Heat** Flow Rate **and Outside Surface Temperature** (Similar to problem solved by Holman, Reference HO-81, pp. 28, 29)

Problem Statement. This problem concerns the steady-state radial temperature distribution and interface temperatures for a series of three concentric cylindrical annular sections. Each section has a unique value of thermal conductivity that is independent of temperature. The temperature is assumed to be a continuous function from one annular section to another (no reduced conductance region between sections). There is a known steady radial heat flow rate and a known constant temperature at the outside surface of the outermost annular section. A sketch of the geometric configuration is shown in Figure 2.2-1

The governing equation in region c  $(r_3 < r < r_4)$  is

$$
\frac{d}{dr} (r \frac{dT}{dr}) = 0
$$

and the boundary conditions are

 $r = r_a$   $T = T_a$ 

(9) <sup>16</sup>

 $(8)$ 

 $\mathfrak{c}$ 



### **Figure 2.2-1**

Three Concentric Cylindrical Annuli a, b, and c in Which the Temperature Distribution Is to Be Determined for Known emperature Distribution is to be betermined for<br>
Volumetric Heat Generation Rate q''' in the Region (0 r rw) and Known Value of Surface Temperature T4

$$
r = r_3 \qquad Q = -k_c \qquad 2 \qquad r_3 \frac{dT}{dr}
$$
\nwhere  
\n
$$
T = \text{temperature} \qquad [0]
$$
\n
$$
r = \text{radial position} \qquad [\ell]
$$
\n
$$
r_4 = \text{outside radius of region c} \qquad [\ell]
$$
\n
$$
r_3 = \text{inside radius of region c} \qquad [\ell]
$$
\n(10)

 $k_c$  = thermal conductivity of material of region c [e/t£0]

 $\ell$  = length of cylinder  $[\ell]$ 

 $2 =$  length of cylinder (the analysis could be done on a per unit length basis as it is one-dimensional)  $[2]$ 

 $Q =$  heat flow radially out through the section [e/t]

The heat flow rate to the hollow cylinder at steady-state is related to the heat generation rate per unit volume within the waste region of radius rw by

$$
Q = q''' \pi r_w^2 \ell
$$

(11)

where

 $q'''' =$  volumetric heat generation rate in the<br>waste region  $[e/t^{0.3}]$ waste region  $r_w$  = outside radius of cylindrical waste region [2]

The same differential equation applies to regions b and a. After the equation is solved within region c,  $T_3$  at  $r = r_3$  is known, and the boundary conditions for region b are

 $r = r_3$  T = T<sub>3</sub> (12)

$$
r = r_2
$$
  $Q = -k_b 2\pi r_2 \frac{\mu dT}{dr}$   $r = r_2$  (13)

Similarly, after the solution is obtained in region b,  $T_2$  at r =  $r_2$  is known. The boundary conditions for region a are

$$
r = r_2 \qquad T = T_2
$$
\n
$$
r = r_1 \qquad Q = -k_a \ 2 \pi r_1 \frac{\rho dT}{dr} \Bigg|_{r = r_1}
$$
\n(14)

Objectives. The solution can be compared to a WAPPA thermal model solution for a waste package with engineered barriers.

Analytical Solution. The analytical solution for the continuous temperature distribution is

$$
T = T_{4} + \frac{q' \cdot r_{w}^{2}}{2k_{c}} \ln \frac{r_{a}}{r} \qquad (r_{3} \leq r \leq r_{4})
$$
\n
$$
T = T_{3} + \frac{q' \cdot r_{w}^{2}}{2k_{b}} \ln \frac{r_{3}}{r} \qquad (r_{2} \leq r \leq r_{3})
$$
\n(16)

$$
T = T_2 + \frac{q''r_w^2}{2k_a} \ln \frac{r_2}{r} \qquad (r_1 \le r \le r_2)
$$
 (18)

The surface temperature values are

$$
T_3 = T_4 + \frac{q'' + r_w^2}{2k_c} \ln(\frac{r_4}{r_3})
$$

(19)

$$
T_2 = T_3 + \frac{q^{11}r_w^2}{2k_b} \ln(\frac{r_3}{r_2})
$$

$$
T_1 = T_2 + \frac{q''r_w^2}{2k_a} \ln(\frac{r_2}{r_1})
$$

#### Assumptions.

- Each region has a unique value for thermal conductivity that is independent of temperature.
- The axial heat conduction and temperature gradient are negligible in comparison to the radial.
- The temperature is continuous from one annular region to another (no reduced conductance region between regions).

Input Specifications. (Similar to defense high level waste cast steel overpack, see Reference ON-83, pp. 33, 159)

- Geometry (see Figure 2.2-1)
	- radii

waste region outer radius region a inner radius = **r.** region a outer radius =  $r_2^+$ region b outer radius =  $r\frac{2}{3}$ region c outer radius = r I i I = rw = 30.5 (cm) = 30.5 (cm) = 43.0 (cm) = 54.0 cm = 65.0 cm

Material properties

thermal conductivity

region a value = k<sub>a</sub> = 53.4 (w/m<sup>o</sup>C) region b value = k $\bar{\mathsf{b}}$  = region c value = k<sub>C</sub> = 54.5 55.6 (w/moc) (w/moc)

Boundary conditions

```
region c outside temperature = T_a = 170 (<sup>O</sup>C)
waste region volumetric heat generation
rate = q^{i+1} = 0.001315 (w/cm<sup>3</sup>)
```

$$
(21)
$$

(20)
Output Specifications. The region a, b, and c boundary temperatures  $T_1$ ,  $T_2$ , and  $T_3$  are to be determined. These values can be compared with the values given below.



### **2.3** Transient Temperature Response of a Solid Cylinder with Constant Thermal Conductivity

Problem Statement. This problem is concerned with the thermal response of an infinite solid cylinder (radial conduction only) of radius a, initially at a uniform temperature  $T_i$  which is equal to the atmospheric temperature. The atmospheric temperature is suddenly changed to a constant value of  $T_f$ . Subsequent to this change at time zero, the change in the temperature distribution in the cylinder is to be calculated with time. See Figure 2.3-1.

The energy conservation equation for only transient radial conduction in the region  $(0 \le r \le a)$  is

$$
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) = \frac{1}{\alpha} \frac{\partial T}{\partial t}
$$
 (22)

where the thermal conductivity is considered to be invariant and where

$$
T = temperature
$$
 [0]  
\n $r = radial position$  [2]  
\n $t = time$  [t]  
\n $\alpha = thermal diffusivity$  [2/t]





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 $(c)$   $t > 0$ 

Cylinder of Radius a Initially in Temperature Equilibrium with Surrounding Atmosphere at Temperature T<sub>i</sub>. At Time Zero the Surrounding Atmospheric Temperature Is Increased to a Value  $T_{\rm g} = T_f$ 

At the surface of the cylinder, heat may be convected between the cylinder and the atmospheric fluid. The characteristic temperature of the atmospheric fluid is  $T_{\infty}$ . The initial condition is

(23)

(24b)

$$
t < 0 \qquad T(r) = T_i \qquad (0 \leq r \leq a)
$$

and the surrounding atmospheric temperature is

$$
t < 0 \quad T_{\infty} = T_{\text{i}}
$$
\n
$$
t \geq 0 \quad T_{\infty} = T_{\text{f}}
$$
\n
$$
(24a)
$$

The boundary conditions are

at 
$$
r = a
$$
,  $-k \frac{\partial I}{\partial r} = h(T - T_{\infty})$  (25)  
at  $r = 0$ ,  $\frac{\partial T}{\partial r} = 0$  (26)

where

k = thermal conductivity of cylinder material [e/ttel

h = convective heat transfer coefficient between the cylinder outer surface and the atmosphere  $[e/t\ell^2\theta]$  Objectives. The purpose of this problem is to establish a reference solution for transient radial conduction in a cylinder. It will be representative of waste package transient cooling when there is an abrupt change in atmospheric conditions. The solution applies to thermal conditions where the associated thermal stresses may be important.

Analytical Solution. The solution to Equation 22 for the stated initial and boundary conditions (Reference CA-59) is

$$
\frac{T(r,t) - T_{\infty}}{T_{i} - T_{\infty}} = \frac{2ha}{k} \sum_{n=1}^{\infty} \frac{e^{-d\lambda_{n}^{2}t}}{\left[\lambda_{n}^{2} a^{2} + (\frac{ha}{k})^{2}\right]} J_{o}(\lambda_{n}a)
$$
\n(27)

where  $\lambda_n$  are the characteristic values found from solving

$$
(\lambda_n a) J_1(\lambda_n a) + (\frac{ha}{k}) J_0(\lambda_n a) = 0
$$
\nand wh.  
\n
$$
J_i \wedge \lambda_n \omega
$$
\nf first kind and order  
\nt variable y  
\n
$$
J_i
$$
\n
$$
J_i
$$
\n
$$
f \text{ first kind and order}
$$
\none of independent variable y

This analytical solution involves evaluation of the terms of an infinite series until the terms of the convergent series become negligible. A more rapid solution can be obtained by the use of charts developed by Heiser (Reference HE-47), Boelter et al. (Reference BO-42), and Kreith (Reference KR-58). These charts are shown in Figure 2.3-2. They treat  $r/r_a$  from O to 1.0 in increments of 0.2 (six charts). Each chart presents 11 combinations of values of  $k/h_a$  in the range from 0 to 10.



Figure 2.3-2

Dimensionless Temperature Distribution in a Long Circular<br>Cylinder Subjected to a Sudden Change in<br>Environmental Temperature

#### Assumptions.

- The surface convection heat transfer coefficient  $\bullet$ is a known constant.
- The atmospheric temperature is constant for  $t > 0$ and therefore independent of the thermal energy transferred to the cylinder.
- Thermal conductivity and thermal diffusivity are independent of temperature and thus constant through the transient.

### Input Specifications.

- **Geometry** 
	- $cylinder$  radius,  $a = 1.0$  (ft)
- Material properties
	- thermal diffusivity of cylinder material,  $\alpha = 0.014$  (ft<sup>2</sup>/hr)
	- thermal conductivity of cylinder material,  $k = 0.700$  (Btu/hr-ft-<sup>OF</sup>)
- **Parameters** 
	- convective heat transfer coefficient,  $h = 2.8$  (Btu/hr-ft<sup>2</sup>-<sup>0</sup>F)
- Boundary conditions
	- initial temperature of cylinder and pre-step
	- $(t \le 0)$  atmospheric temperature,  $T_i = 300($ OF)
		- $post$  step (t > 0) atmospheric temperature,
		- $t_f = 400$  (OF)

Values of temperature as a function of radial position and time are given in the following table in terms of the thermal and geometric parameters:



For this problem, the first six roots of Equation 28,  $\lambda_n$  are:



Summations using the first two roots in Equation 27 will give values of temperature accurate to 0.010C.

Output Specifications. This problem solves for the temperature response as a function of radius and time. The solution can be compared with the values in the preceding table.

27

### 2.4 One-Dimensional Transient Temperature Distribution with Phase Change

Problem Statement. This problem simulates the transient temperature response of a fluid initially at OOC as one wall is lowered to a temperature of -450C causing a freezing interface to propagate into the liquid. Temperatures are to be calculated as a function of time and distance from the surface boundary. The purpose of this problem is to provide a basis for examining the modeling assumptions and algorithms used by codes for the calculation of temperatures during phase changes for materials with significant latent heats.

Physical Description. A one-dimensional slab is occupied by a liquid at 0°C. At the beginning of the transient ( $t=0$ ), the edge is instantaneously lowered to a temperature of -45°C. The freezing temperature of the liquid is  $-0.01$ <sup>O</sup>C. As heat is removed from the liquid, the freezing front propagates away from the cold surface and into the liquid (see Figure 2.4-1).

Problem Solution. Conductive heat transfer with phase change is governed by the following differential equation

$$
k \frac{\partial^2 T}{\partial x^2} = \rho c \frac{\partial T}{\partial t} + L
$$

(29)

where

- $T =$  temperature and the units of temperature are  $[0]$
- $x = position measured into the solid/fluid region$ from the cold edge  $[\ell]$

 $p =$  mass density of the fluid and of the solid  $[m/\ell^3]$  $c =$  specific heat of the fluid and of the solid  $[e/m]$  $k =$  thermal conductivity of the fluid and of the solid  $[e/tk]$  $L =$  heat of fusion [e/ $\ell^{3}$ ]

28





where  $t_{max}$  is the maximum time to be analyzed

## Figure  $2.4-1$

Slab from Semi-Infinite Freezing Liquid with<br>One Boundary at  $T = -45$ OF

Reference CA-59 provides a solution for this problem of:

$$
T(x,t) = T_0 \left(1 - \text{erf}\left[\frac{x}{2(at)^{1/2}}\right] / \text{erf}(\lambda)\right) \text{ for } x < 2\lambda(at)^{1/2}
$$
  

$$
T(x,t) = T_1 \qquad \text{for } x \ge 2\lambda(at)^{1/2}
$$

where

 $T(x,t)$  = temperature

 $x = distance from the boundary$ 

 $t = t$ ime

 $T_1$  = initial temperature of the liquid

 $T<sub>o</sub>$  = boundary temperature

 $a =$  thermal diffusivity ( $a = k/pc$ )

 $\lambda$  = an equation parameter that satisfies

$$
\lambda e^{\lambda^2} \text{erf}\lambda = \frac{C(T_1 - T_0)}{\ln^{1/2}}
$$

$$
c =
$$
specific heat

 $p = density$ 

 $k =$  thermal conductivity

 $L =$  heat fusion

Table 2.4-1 provides a list of values of the parameter  $\lambda$  as a function of specific heat, temperature difference, and latent heat. When the value of  $\lambda$ is relatively small ( $\lambda \leq 0.2$ ), it can be approximated by

$$
\lambda^2 = C(T_1 - T_0)/2L
$$

Assumptions. In modeling the problem, it can be assumed that at a point 200 centimeters into the fluid undergoing the phase change, the temperature remains constant at the initial fluid temperature.

The following input parameter values should be used:

k = 528 cal/cm sec **OC**  $P = 0.92$  g/cm<sup>3</sup>  $c = 0.48$  cal/g <sup>O</sup>C  $a = 1196$  sec.cm<sup>2</sup>  $L = 144 \text{ cal/g}$  $T_1 = 0$ <sup>o</sup>C  $T_0$  = -450C  $C(T_1 - T_0)$  $\sqrt{1/2}$  = 0.0846  $\lambda = 0.267$ 

Calculated results can be compared with the values in Table 2.4-2.

Output Specifications. The outputs for this problem are the temperature as a function of time and distance. The temperatures are to be calculated at positions 1, 2, 5, 10, 20, 50, and 100 centimeters from the boundary at times of 0.25, 0.5, 1, 2, 5, 10, 20, 50, and 100 seconds.

## Table 2.4-1

Values of the Parameter



 $\ddot{\phantom{a}}$ 

## Table 2.4-2

### Time-Dependent Temperature Distribution in a One-Dimensional Slab Undergoing Phase Change



## Table 2.4-2 (continued)



### **2.5 Hypothetical Problem to** Simulate the **Steady-State Temperature Distribution in a Waste Package**

Problem Statement. This problem is intended as an extension of Cases 2.1 and 2.2 to include the waste region and an arbitrary number of annular regions. It can be used to determine the steady-state radial temperature distribution in a series of n concentric hollow cylinder (annular sections) which:

- Surround a solid cylinder with a spatially uniform heat generation rate, representative of the waste form
- Have regionally varying values of thermal conductivity
- Have interfaces with a common temperature value (there is no high thermal resistance at the interface between regions). Similarly, the interface between the solid cylinder and the smallest hollow cylinder has a unique value of temperature (no high thermal resistance acts at an interface).

The radial heat flow rate across a cylindrical surface of a radius within the range of radii of the hollow cylinders can be determined algebraically from the outside dimension of the solid cylinder and its volumetric heat generation rate. This algebraic relationship is used along with Fourier's law for conduction to obtain a boundary condition at the inside surface of each annular section in terms of the temperature gradient at that radius. Also, a known temperature exists at the outer surface of the largest annular section. Solutions for the temperature distribution are obtained progressively from the largest annular section to the smallest. For the solid section, the boundary conditions are:

- The temperature on the outside surface is known
- The radial temperature gradient at the center is zero

A sketch of the geometric configuration is shown in Figure 2.5-1.



## Figure 2.5-1

N Concentric Cylindrical Annuli with Known Outside Temperature T<sub>O</sub>,<br>Surrounding a Waste Region of Radius  $r_w$  in Which a Known Volumetric<br>Heat Generation Rate of q''' Exists. Each Region Can Have a<br>Unique But Constant Th

For each of the n annular regions, the governing equation is For each of the n annular regions, the governing equation is

$$
\frac{d}{dr} \left( r \frac{dI}{dr} \right) = 0 \tag{30}
$$

in terms of the general region j where  $(r_i^j \le r \le r_0^j)$ . The boundary conditions are:

$$
r = r_0^{j} \qquad T = T_0^{j}
$$
\n
$$
r = r_j^{j} \qquad Q = -k^{j} \quad 2\pi \quad r_j^{j} \quad \frac{dI}{dr} \Big|_{r = r_j}^{j}
$$
\n(31)

 $(32)$ 

where

 $T =$  temperature

 $r =$  radial position

 $r_i$ <sup>j</sup> = inside radius of j<sup>th</sup> annular region

- $r_0$ j = outside radius of j<sup>th</sup> annular region<br>
k<sup>j</sup> = thermal conductivity of material of region j<br>  $\ell$  = length of cylinder (the analysis could be done<br>
on a per unit length basis as it is one-dimensional)
	- $Q$  = heat flow radially out through the section

The heat flow rate through each hollow cylinder at steady-state is related to the heat generation rate per unit volume within the waste region of radius  $r_w$  by

$$
Q = q'''' \pi r_w^2 \ell
$$

(33)

where

- $q''''$  = volumetric heat generation rate in the waste region  $(0 \le r \le r_w)$  $r_w$  = outside radius of cylindrical waste region  $\ell$  = length of cylindrical waste region
- The same differential equation and boundary conditions apply to all annular regions. After a solution is obtained for region j, the temperature at  $T_i$ <sup>j</sup> is evaluated and

$$
T_0j^{+1} = T_jj
$$

(34)

is used as the boundary condition for region j+l.

For constant thermal conductivity, the differential equation expressing the energy conservation principle in the waste region  $(0 < r < r_w)$  is

$$
\frac{d}{dr} \left( r \frac{dT}{dr} \right) + \frac{q'' + r}{r^W} = 0
$$

**k** (35)

where

**kw=** thermal conductivity of the waste region

and the other symbols are as previously defined. The mathematical statement of the boundary conditions is:

$$
r = r_{w} \qquad T = T_{i}^{n}
$$
\n
$$
r = 0 \qquad \frac{dT}{dr} = 0
$$
\n(36)

where  $T_i^n$  is known from evaluating the last solution obtained for annular region n.

Objectives. This problem is useful in representing a multi-region waste package including the waste and the engineered barriers. It can be used to evaluate WAPPA multi-region thermal analysis capabilities. Also, it can be used to evaluate ANSYS and HEATING thermal analysis methods.

Analytical Solution. For the j<sup>th</sup> annular region where  $1 \leq j \leq n$ , the solution for the continuous temperature distribution in that region ( $r_i$ )  $\leq$  $r < r_0$ j) is

$$
T = T_0^{\ j} + \frac{q''{r_w}^2}{2k^{\ j}} \quad \text{on } \frac{r_0^{\ j}}{r}
$$
 (38)

which can be evaluated at the inside radius of the j<sup>th</sup> region,  $r = r_i j$ , to give

$$
F_{i}^{j} = T_{0}^{j} + \frac{q^{11}r_{w}^{2}}{2k^{j}} \ln \frac{r_{0}^{j}}{r_{i}^{j}}
$$

(39)

where all terms on the right side are known. By using Equation 34 and incrementing j in Equations 38 and 39, the temperature distribution in the j+l<sup>th</sup> region and the temperature at the inside surface of the j+l region can be determined.

The solution to Equation 35 for the temperature distribution in the waste region ( $0 < r < r_w$ ) for the boundary conditions of Equations 36 and 37 is:

$$
T = T_1^{n} + \frac{q^{n}}{4k^{w}} (r_{w}^{2} - r^{2})
$$

(40)

(41)

and the maximum temperature occurs at  $r = 0$  and is

$$
T_{\text{max}} = T_i^W = T_i^n + \frac{q''{r_w}^2}{4k^W}
$$

where all terms on the right side of Equation 39 are known.

#### Assumptions.

- Each region has a unique value of thermal conductivity that can be specified at the beginning of the problem and is constant throughout the region.
- The axial heat conduction and temperature gradient are negligible in comparison to the radial.
- The heat generation is uniform throughout the waste region.

### Input Specifications.

- Geometry (see Figure 2.5-1)
	- radii (for  $n = 7$ )

$$
r_0^6 = r_1^7 = 60. \text{ (cm)}
$$
\n
$$
r_0^5 = r_1^6 = 55. \text{ (cm)}
$$
\n
$$
r_0^4 = r_1^5 = 50. \text{ (cm)}
$$
\n
$$
r_0^3 = r_1^2 = 45. \text{ (cm)}
$$
\n
$$
r_0^2 = r_1^3 = 40. \text{ (cm)}
$$
\n
$$
r_0^1 = r_1^2 = 35. \text{ (cm)}
$$
\n
$$
r_1^1 = r_0^w = 30.5 \text{ (cm)}
$$
\n
$$
r_1^w = 0
$$

Material Properties

- thermal conductivity  
\n
$$
k^{7} = 51 \text{ (w/m0C)}
$$
\n
$$
k^{6} = 52 \text{ (w/m0C)}
$$
\n
$$
k^{5} = 53 \text{ (w/m0C)}
$$
\n
$$
k^{4} = 54 \text{ (w/m0C)}
$$
\n
$$
k^{3} = 55 \text{ (w/m0C)}
$$
\n
$$
k^{2} = 56 \text{ (w/m0C)}
$$
\n
$$
k^{1} = 57 \text{ (w/m0C)}
$$
\n
$$
k^{w} = 1.0 \text{ (w/m0C)}
$$

Boundary conditions

- Largest annular region outside temperature **=** T<sub>o</sub><sup>7 =</sup> 170 (<sup>o</sup>C
- Waste region volumetric heat generation rate =  $q^{111}$  = 0.001315 (w/cm<sup>3</sup>)

<u>Output Specifications</u>. The temperatures at  $r = 0$ ,  $r_i^1$ ,  $r_i^2$ ,  $r_i^3$ ,  $r_i^4$ ,  $r_i^5$ ,  $r_i^6$ , and  $r_i^7$  are to be determined.

Temperatures determined using the analytical solution from Equations 39 and 41 are given in Table 2.5-1.

### Table 2.5-1



# Analytical Solution for Temperature Distribution

42

### **2.6 Hypothetical Radial Heat Transfer Analysis of** PWR **Fuel Assembly in a Vertical Canister**

Problem Statement. A series of tests has been conducted to measure the thermal response of 12-foot-long PWR fuel assemblies in a vertical cylindrical canister. The tests were conducted at the Engine Maintenance, Assembly and Disassembly (E-MAD) facility on the Nevada Test Site.

A single PWR fuel assembly was enclosed in a 0.375 inch thick canister, with a 14-inch outside diameter, made from 304 stainless steel pipe. An elevation view of the canister is shown in Figure 2.6-1. The cross section of the fuel assembly section is shown in Figure 2.6-2.

Objectives. It is intended that the steady-state radial temperature profile be determined. The boundary conditions and fuel canister loading are similar to those that may exist in a high-level waste repository.

Analytical Solution. The problem will be used to assess the ability of an analysis program to represent and simulate conditions encountered in the field. No analytical solution is available.

Input Specifications. The dimensions of the canister are shown in Figure 2.6-1. The canister is fabricated from 304 stainless steel. Separate cases are provided for different fuel assembly powers, canister outside temperatures, and fill gases. Tables 2.6-1 and 2.6-2 summarize the conditions under which data have been gathered. Fuel assembly thermal output as a function of time is given in Figures 2.6-3 and 2.6-4.

The thermal properties, including thermal conductivity and surface emissivity, will be taken from the waste package data summary report.

Output Specifications. Temperatures at thermocouple locations given in Figures 2.6-5 and 2.6-6 and Table 2.6-3 will be determined and compared with measured values given in Tables 2.6-4 through 2.6-15 and Tables 2.6-16 through 2.6-27.

43



Figure 2.6-1

 $\overline{\phantom{a}}$ 

Elevation View of PWR Fuel Assembly Loaded into Canister





Cross-Section View of PWR Fuel Assembly Loaded into Canister

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## Fuel Assembly 43 Temperature Test Summary



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 $\mathcal{A}^{\mathcal{A}}$ 

 $\ddot{\phantom{1}}$ 

## Fuel Assembly D15 Temperature Test Summary



\*Test backfill was not vacuum; data therefore not included



### Figure 2.6-3

Canister Thermocouple Locations



**Figure 2.6-4** 

Comparison of Calorimetry Data with Predicted Decay Heat<br>Curve for Fuel Assembly B43



**Figure 2.6-5** 

Comparison of Calorimetry Data with Predicted Decay Heat<br>Curve for Fuel Assembly D15





Canister Lid Thermowell Tube Identification<br>(Top View of Lid)



 $\overline{a}$ 



\* See Figure 2.6-6 for illustration of thermowell locations

\*\* Connected to heater controller C21

<sup>†</sup> Electrical check showed low internal resistance - readings may be in error

### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: B43

 $\ddot{\phantom{a}}$ 





### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: B43



#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: B43

55

 $\ddot{\phantom{a}}$ 

#### Fuel Assembly Internal Temperature Measurement **Test** Thermocouple Data Fuel **Assembly:** B43



DATE: 2/11/80 TEST CONDITIONS: Uniform Canister Temperature TIME: :00 **a..** at **300F** With Yacuum


#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: B43

DATE: 1/14/80 **TIME: 10:30 a.m.** 

÷,



- -





#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: B43

60



#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: B43

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#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: **B43**

 $\sim$ 

### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: B43



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#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: D15

 $\ddot{\phantom{a}}$ 

#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: D15

DATE: 10/27/80 DATE: 10/27/80<br>TEST CONDITIONS: Uniform Canister Temperature at 400°F With Heliu



 $T_{\rm eff}$ 

#### test Conditions: University Canadian Canadian Canadian Canadian Canadian Canadian Canadian Canadian Canadian C  $TIME: 4:00$ The Conditions: Unitern Canister Tea Teupt"F) T/C No. 1 = 1/C No.<br>362 529.6 428<br>361 531.5 427  $Temp(°F)$ T/C No.  $Temp(°F)$ 529.6  $428$ <br> $427$  $393.3$  $492$ <br> $491$ 418.2 531.5 402.0 09.4  $360$   $536.2$  $426$ <br> $425$ 400.0 402.0<br>400.0 490 359 534.5 489 358 535.2 424 488  $357$   $532.2$ <br> $357$   $52.5$ 423 487 98.9<br>165.0  $422$ <br> $421$ 486  $355$ <br>355<br>364.6 536.6 396.6 485 148.7  $420$ <br> $419$ 484 132.4 335.0<br>353 537.6<br>352 530.3 407.6 483  $\frac{1}{2}$ 399.1 418 482<br>481 350 525.0<br>35) 520 7 369.6 417 399.1<br>369.6 350 325.0<br>349 525.0<br>348 529.3 238.9 416 480 165.5 371.5 415 479 409 374.3 478 329.8 347<br>347 532.2<br>346 536.4 237.7<br>329.8 408 340.4 374.3<br>340.4 477  $\frac{407}{406}$ 476<br>475 329.2 330.0<br>345 536.4<br>344 537.3 468.4 **"4** 404.4 329.2<br>404.4 500.9 405 474<br>473 344 537.3<br>389.0 403.1  $\begin{array}{@{}ll@{}} 343 & 525.1 \\ 342 & 489.0 \\ 341 & 532.2 \\ 340 & 533.3 \end{array}$ 404  $\frac{3}{5}$ 505.5 403 503.5<br>505.5 472 341 532.2<br>340 533.3<br>339 536.6<br>338 536.6<br>337 537.7 402 471 401 504.4 470 364.7  $\begin{array}{r} 339 \\ 339 \\ 338 \\ 337 \\ 337 \\ 336 \\ 337.7 \\ 336 \\ 336.8 \\ 337.7 \\ 336 \\ 336.4 \\ 398.4 \\ 399 \end{array}$  $400$ <br> $399$ 469<br>468<br>467 364.1 504.4 364.7<br>364.1 482.3 497.3 398 348.2 397 518.1 343.7 466 396 518.8 465<br>464 340.5 332 537.5 394 343.7<br>340.5<br>329.9 395 520.8 ази — эээ.о<br>332 — Бат Е 394 523.6 336 537.3<br>331 = 537.6 463 393 507.1 462 329 537.3<br>330 537.9 335.8<br>337.4 392  $\frac{1}{2}$ 461 328 337.6<br>328 525.3 329 525.3<br>328 465.5  $391$ 316.2 460  $390$ 506.5 459<br>458 327 502.3<br>327 501.1 389 506.5 *325* 507.7 387 320.0<br>330.3 388 325 506.8 3866.<br>325 507.3 457 509.6 509.4<br>509.6 387  $324$  507.1<br>324 506.3 456 386 455 385 495.1 303.1 321 477.1 383 320 516.9 382 454 384 529.0 323.2 453 303.1<br>323.2 533.6 383 319 517.0 381 451 535.7  $382$ 318 518.3<br>318 517.0 450  $381$ <br> $380$ 536.5 535.7<br>536.5 317 517.0<br>318 522.3 449 340.3 316 522.3 378 448 379 535.7 351.8 447<br>446 316<br>31652.3<br>31652.1 521.5 378 375.3 522.4 526.7 377 313 511.3<br>314 460.8 445 314 469.4<br>313 503.1 376 444 535.1 375 443 311 505.4 373 386.3<br>376.3  $\begin{array}{@{}c@{\hspace{1em}}c@{\hspace{$ 374 442 535.5 373 309 506.3 371 <sup>308</sup>497.7 <sup>370</sup> 441 368.2<br>370.9  $\frac{372}{371}$ <br> $\frac{370}{370}$ 524.1 440 437<br>436  $303$ <br>308 497.7<br>307 500.5<br>306 545.5<br>305 546.2 435 369 435 S37.5 403.8 368 434 537.9 367 408.3  $303$   $557.4$ <br> $303$   $557.4$ 433 403.8<br>408.3 536.9 366 432 365 **483.4** 303 530.3<br>309 Fee C 431 364 430

# Fuel Assembly Internal Temperature Measurement Test Assembly Internal Temperature Measur

429

 $392.1$ 

363

 $301$ 

544.0



DATE: 11/5/80 TIME: 8:00 a.m.



#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: D15



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J.

J.





#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: **D15**

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#### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: **D15**



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### Fuel Assembly Internal Temperature Measurement Test Thermocouple Data Fuel Assembly: **D15**

76

#### 2.7 Hypothetical Calculation of Canister Temperature Distribution Subsequent to Being Filled with a Hot Glass Waste Form

Problem Description. Under some heat transfer conditions, large temperature gradients can exist. These temperature gradients can impose large internal loads on the structure due to the structure's inherent constraint of the accompanying thermal expansion. The design and performance assessment of canisters into which molten glass waste is poured must be analyzed to determine the temperature distribution. The temperature distribution will subsequently be used to evaluate the stress distribution. Since the heat transfer process is a transient one, its response will need to be monitored at various discrete values of time so that it is likely that approximately the worst stress conditions will be monitored. A sketch of the waste canister into which the molten glass is assumed to be poured is shown in Figure 2.7-1.

Objectives. The objectives of this problem solution are to obtain the temperature distribution in a canister for various times subsequent to the thermal shock of being filled with a molten glass waste form. The temperature distribution conditions will be used to analyze corresponding thermal stress distributions.

Analytical Solution. This is a hypothetical problem for which computer program modeling will be conducted and the simulated response obtained. It is expected that ANSYS will be used. An analytical solution other than that from the computer program model will not be determined.

#### Assumptions.

- The molten waste form is poured instantaneously into the canister at time zero.
- The thickness of the canister walls is  $0.5$  cm.
- The atmosphere is at a fixed temperature.

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Canister into Which Molten Glass Waste Form Is Poured

The nuclear decay heat generation can be neglected because the glass is very hot and only the early part of the transient is of interest.

Input Specifications. The canister material is 304 stainless steel. The dimensions are:

 $l =$  length = 300.0 (cm)  $r_i$  = inside radius = 30.0 (cm)  $r_0$  = outside radius = 30.5 (cm)

The molten glass assumed to be poured into the canister instantaneously at the beginning of the transient (at time equals zero) has a temperature of 1000°C. The canister is initially at 800°C. The outside surface of the canister loses heat to the atmosphere which is at a fixed temperature of 3000C according to

$$
q = h(T_0 - T_a)
$$

where

- $q$  = heat transfer rate per unit area (w/m<sup>2</sup>)
- h = heat transfer coefficient between canister and atmosphere (w/m2oC)
- $T_0$  = outside temperature of canister (OC)
- $T_a$  = fixed temperature of atmosphere which serves as a heat sink =  $300.0$  (<sup>O</sup>C)

The free convection heat transfer coefficient between the outside surface of the canister and the atmosphere is given by

h =  $0.25(T_0 - T_a)^{0.25}$ 

The following glass properties will be used:

l.



The following 304 stainless steel conduction properties will be used:



Output Specifications. The analyst must monitor the temperature distributions at various times and choose those that are most severe as the thermal load cases for the subsequent stress analyses.

 $\ddot{\phantom{a}}$ 

#### **3.0 MECHANICAL** ANALYSIS PROBLEMS

Problems included in this section have been selected to test the mechanical or stress aspects of waste package codes against analytical solutions or hypothetical problems. Specific processes that must be tested in waste package performance assessment codes include:

- Linear-elastic displacements
- Elastic-plastic displacements
- Creep
- Thermal-induced stresses
- Dynamic displacements due to handling accidents or normal transportation loads
- Geometric instability (buckling)
- Creep buckling

Not all of the above processes can necessarily be analyzed using one code. The testing of the code may therefore involve analyzing two or three of the problems developed for relatively simple codes or up to six or seven for the more complex codes.

#### 3.1 **Radial and Tangential Stress Components at the** Inner **and Outer Surfaces of** a **Thick-Walled Cylinder with** a **Radial Temperature Profile**

Problem Statement. This problem concerns the radial and tangential stress components at the inner and outer surfaces of a hollow cylinder  $(r_i \le r \le r_0)$ , which suppports a radial temperature distribution

$$
T(r) = T_0 + \frac{q''r_w^2}{2k} \text{ in } (r_0/r)
$$

(42)

as given in thermal problem 2.1. In this equation

 $r =$  radial position  $r_i < r < r_0$  [2]

 $r_i$  = inside radius of hollow cylinder  $\lbrack l \rbrack$ 

 $r_0$  = outside radius of hollow cylinder [U]

- $r_w$  = outside radius of solid cylindrical region in which volumetric heat generation  $q'$   $'$  applies  $r_i \leq r_w$  [2]
- $k =$  thermal conductivity of hollow cylinder material (assumed constant)  $[e/t\ell\theta]$ (assumed constant)
- $q''''$  = uniform volumetric heat generation rate in solid cylindrical region of outer region  $r_w$  [e/t $\ell^{3}$ ]
	- $T_0$  = temperature of outer surface of hollow cylinder at  $r = r_0$  [ $\theta$ ]

Objectives. The solution to this problem can be used to verify the accuracy of the WAPPA and ANSYS structural analysis models. The verification is directed to the treatment of the radial temperature distribution and the structural response, in terms of the radial and circumferential stress components that it causes.

Analytical Solution. The general solution given by Timoshenko (TI-56) for the radial stress component at any position  $r_1 \le r \le r_0$  where the radial stress is zero on the inside and outside surfaces is

$$
\sigma_{r} = \frac{E}{1-v} \left[ -\frac{1}{r^{2}} \int_{r_{i}}^{r} \alpha T(r) r dr + \frac{r^{2} - r_{i}^{2}}{r^{2}(r_{0}^{2} - r_{i}^{2})} \int_{r_{i}}^{r_{0}} \alpha T(r) r dr \right]
$$
(43)

and the circumferential stress component is given by

$$
\sigma_{t} = \frac{E}{1-\nu} \left[ \frac{1}{r^{2}} \int_{r_{i}}^{r} \alpha T(r) r dr + \frac{r^{2} + r_{i}^{2}}{r^{2}(r_{0}^{2} - r_{i}^{2})} \int_{r_{i}}^{r_{0}} \alpha T(r) r dr - \alpha T(r) \right]
$$
(44)

where

E = material's elastic modulus  $[f/g^2]$  $v =$  material's Poisson's ratio  $\begin{bmatrix} 1 \end{bmatrix}$  $\alpha$  = material's coefficient of thermal expansion [l/ $\theta$ ] r = general radial position in the range  $r_i$  <  $r$  <  $r_0$  [*g*]  $r_i$  = inside radius of hollow cylinder  $[\ell]$  $r_0$  = outside radius of hollow cylinder [2]  $\sigma_r$  = radial stress component [f/ $\ell^2$ ]  $\sigma_t$  = circumferential stress component [f/ $\ell^2$ ]  $T(r)$ = temperature at position r ( $r_i < r < r_0$ ) in the hollow cylinder [e]

Figure 3.1-1 shows the solid cylinder configuration in which the heat is generated and the larger concentric hollow cylinder for which the radial and tangential thermal stress components will be analyzed.

Using Equation 42 for the temperature distribution

$$
T(r) = T_0 + \frac{q''r_w^2}{2k} \ln(r_0/r)
$$

(42)



# **Figure 3.1-1**

Hollow Cylinder rists with Steady-State Radial Temperature Distribution for-Which Radial and Tangential Stress Components Will Be Analyzed

and for  $k = constant$ , the integrals are

$$
\int_{r_{\rm i}}^{r} \mathsf{T}(r) \, \mathrm{r} \, \mathrm{d}r = \frac{\mathsf{T}_{\rm o}}{2} \left( r^2 - r_{\rm i}^2 \right) + \frac{\mathsf{q}^{\prime \prime \prime} \mathsf{r}_{\rm w}^2}{2k} \left[ \frac{r^2}{2} \left( \ln \frac{r_{\rm o}}{r} + \frac{1}{2} \right) - \frac{r_{\rm i}^2}{2} \left( \ln \frac{r_{\rm o}}{r_{\rm i}} + \frac{1}{2} \right) \right]
$$
\n(45)

and

-

$$
\int_{r_{\mathbf{j}}}^{r_{0}} \mathsf{T}(r) r dr = \frac{\mathsf{T}_{0}}{2} (r_{0}^{2} - r_{\mathbf{j}}^{2}) + \frac{\mathsf{q}^{11} r_{w}^{2}}{2k} \left[ \frac{r_{0}^{2} - r_{\mathbf{j}}^{2}}{4} - \frac{r_{\mathbf{j}}^{2}}{2} \ln \frac{r_{0}}{r_{\mathbf{j}}} \right]
$$
\n(46)

Thus, Equations 43 and 44 can be evaluated to give the radial and tangential stress components for any radial position r for the temperature distribution given by Equation 42.

Equations 43 and 44 can be written as

$$
\sigma_r = \frac{E}{1-\nu} \left[ \frac{(1 - r_i^2/r^2)B}{(r_0^2 - r_i^2)} - \frac{A(r)}{r^2} \right]
$$

(47)

 $\sigma_t = \frac{E}{1-v} \left[ \frac{1 + (r_i/r)^2 B}{(r_0^2 - r_i^2)} + \frac{A(r)}{r^2} - \alpha T(r) \right]$ 

(48)

where

×

ż

$$
B = \frac{\alpha T_0}{2} (r_0^2 - r_1^2) + \frac{q''r_w^2 \alpha}{2k} \left[ \left( \frac{r_0^2 - r_1^2}{4} \right) \frac{r_1^2}{2} \ln \frac{r_0}{r_1} \right]
$$
(49)

and

$$
A(r) = \frac{\alpha T_0}{2} (r^2 - r_1^2) + \frac{q''{r_1}^2 \alpha}{4k} \left\{ r^2 \left[ \ln(\frac{r_0}{r_1}) + 1/2 \right] - r_1^2 \left[ \ln(r_0/r_1) + 1/2 \right] \right\}
$$

(50)

86

and

Equations 47, 48, 49, and 50 can be evaluated to predict analytically the radial distribution of the radially and tangentially directed stress components.

#### Assumptions.

- The thermal conductivity of the hollow cylinder material is constant.
- The coefficient of thermal expansion of the hollow cylinder is constant.
- The material is isotropic

### Input Specifications.

- Geometry
	- waste region radius,  $r_w = 30.5$  (cm)
	- hollow cylinder inside radius,  $r_i = 30.5$  (cm)
	- hollow cylinder outside radius,  $r_0 = 67.5$  (cm)
- Material properties
	- thermal conductivity;  $k = 0.5$  (w/cm<sup>o</sup>C)
	- coefficient of thermal expansion,  $\alpha = 11 \times 10^{-6}$  (1/<sup>o</sup>C)
	- Poisson's ratio;  $v = 0.25$  ()
	- elastic modulus;  $E = 16.2 \times 10^4$  (MPa)

Thermal conditions

- hollow cylinder outside temperature; T<sub>O</sub> = 200(<sup>O</sup>C)
- $\,$  volumetric heat generation rate; q''' = 0.001291 (w/cm<sup>3</sup>)

Equations 47, 48, 49 and 50 have been evaluated at eight radial positions as shown in Table 3.1-1 to determine the radial and tangential stress components at eight values of radius in the range  $(r_i \le r \le r_0)$ .

Output Specifications. The solution to this problem will determine the stress components at the radial positions indicated in Table 3.1-1 using WAPPA and ANSYS.

# Table 3.1-1

Calculated Values of Radial and Tangential Stress Components



### **3.2 Horizontal Simply Supported** Beam **Subjected to Vertical Motion at Both Supports as Defined by a Particular Acceleration Response Spectrum**

Problem Statement. This problem is intended to determine the maximum displacement relative to the supports and the maximum bending stress for the beam shown in Figure 3.2-1. The response spectrum is given in Figure 3.2-2 (Reference BI-64).

Objectives. This sample problem will be used to verify the response spectrum analysis capabilities of structural codes.

Analytical Solution. The fundamental natural frequency of a beam with a uniform mass distribution is given by

$$
f = \frac{\pi}{2g^2} \sqrt{\frac{EI}{m}}
$$

where

 $f =$  vibrational frequency  $[1/t]$  $\ell$  = beam length  $[\ell]$  $E =$  beam material's elastic modulus  $[f/g^2]$ I = beam moment of inertia for in plane bending<br>
(Figure 3.2-1)  $\lceil \ell^4 \rceil$  $(Figure 3.2-1)$  $m =$  beam mass per unit length  $[m/\ell]$ 

Only the first mode given by

 $\phi_1(x) = \sin \frac{\pi x}{2}$ 

(52)

(51)



 $l = 240$  in  $t = 14$  in  $m = 0.2$   $\text{lb}_f$   $\text{sec}^2/\text{ln}$  $EI = 10^{10}$   $Ib_f$ - $in^2$ 



Simply Supported Beam with Support Motion ys(t)



 $\ddot{\phantom{0}}$ 

L.

 $\overline{\phantom{a}}$ 

J.





Maximum Relative Displacement and Maximum Vertical Acceleration Plotted as Response Spectra for Beam Supports Motion

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will be considered where

$$
\phi_1(x) = \text{mode shape} \qquad [1]
$$

The participation factor of that mode in the total motion is given by

$$
r_1 = \frac{\int_0^{\ell} m \phi_1(x) dx}{\int_0^{\ell} m[\phi_1(x)]^2 dx}
$$

(53)

where

 $r_1$  = modal participation factor for the fundamental mode m = beam mass **[ml**  $[ ]$ 

The modal displacement is given by

$$
A_1(t) = \Gamma_1 U_1(t) \tag{54}
$$

where

 $A_1(t)$  = modal displacement for the fundamental mode  $\Gamma_1$  = participation factor of the fundamental mode  $U_1(t)$  = response of the single degree of freedom system  $[2]$ I I  $[2]$
The modal displacement of the distributed mass is

$$
U(t) = \Gamma_1 U_1(t) \phi_1(x)
$$
 (55)

or using Equations 52 and 54

$$
U_1(t) = A_1(t) \sin \frac{\pi x}{g}
$$
 (56)

The maximum bending moment in the beam is given by

$$
M = -EI \frac{\partial^2 u}{\partial x^2}
$$
 (57)

and the maximum bending stress is given by

$$
\sigma = \frac{Mc}{I}
$$
 (58)

where

 $\sigma$  = bending stress [f/ $\ell^2$ ]  $M =$  internal moment by beam cross section at the midspan  $[f - \ell]$  $c =$  beam half thickness in vertical direction  $[\ell]$ I = cross section's moment of inertia  $[2^4]$ 

.These equations allow for the determination of the dynamic response when used in conjunction with the spectra of Figure 3.2-2.

Assumptions. It is assumed that the fundamental mode predominates and the contribution of higher harmonics is negligible.

Input Specifications. As shown in Figure 3.2-1, the beam dimensions and properties are:

```
\n
$$
\ell = length = 240 (in)
$$
\n  
\n $t = height of cross section = 14 (in)$ \n  
\n $m = mass of unit length of beam = 0.2 (lb_f - sec^2/in^2)$ \n  
\n $EI = product of beam elastic modulus and moment of inertia = 1010 (lb_f-in^2)$ \n
```

For this particular case, Equation 51 gives

$$
f = \frac{\pi}{2\ell^2}\sqrt{\frac{EI}{m}} = \frac{\pi^2}{2(240)^2}\sqrt{\frac{10^{10}}{0.2}}
$$

$$
f = 6.1 (cps)
$$

(59)

At a circular frequency of

$$
\omega = 2\pi f = 2(6.1)\pi = 12.2\pi
$$

(60)

the maximum relative displacement  $U_{max}$  from Figure 3.2-2 is

$$
\mathbf{U_1} = 0.44 \text{ (in)}
$$

(61)

Substituting Equation 52 in Equation 53 and integrating, the participation factor for the fundamental mode becomes

$$
\Gamma_1 = 4/\pi
$$

$$
(62)
$$

and from Equation 54

$$
A_{\text{max}} = \frac{4}{\pi} (0.44) = 0.56 \text{ (in)}
$$

(63)

The displacement is then given by Equation 55

 $u(t) = 0.56$  Sin  $\frac{\pi x}{2}$ i

(64)

The maximum bonding moment occurs at the midspan and is given by

$$
M_{max} = \frac{EI\pi^2}{2} A_{max}
$$
  
\n
$$
M_{max} = \frac{10^{10}\pi^2 (0.56)}{(240)^2}
$$
  
\n
$$
M_{max} = 9.6 \times 10^5 \text{ (in-lb)}
$$

(65)

The maximum bending stress in the outer fiber at  $x = \ell/2$  is given by Equation 58

$$
\sigma = \frac{Mc}{I} = \frac{EI\pi^2 c}{\ell^2 I} A_{\text{max}}
$$

$$
\sigma = \frac{(30 \times 10^6)\pi^2 (7) (0.56)}{(240)^2}
$$

$$
\sigma = 20,100 (1b/in^2)
$$

(66)

Output Specification. The output should determine the natural frequencies and the maximum displacement at the center of the span in terms of the internal moment and the bonding stress using a finite element structural analysis program which offers modal summation analysis capabilities.

### 3.3 A Mass Supported by a Thin Rod and Subjected to a Step Load Causing Tension in the Rod and Plastic Deformation

Problem Statement. A mass supported by a thin rod is subjected to a step load which imposes a tensile load in the rod and causes it to experience elastic strain followed by plastic tensile strain. Figure 3.3-1 shows a mechanical model of the structure and the loading history.

Objectives. The objective of this analysis is to determine the displacement transient of the mass and the time when the displacement is at its maximum.

Analytical Solution. The ramp portion of the response when the rod is strained elastically as represented by the spring elongation is regarded

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Figure 3.3-1

(a) Mechanical Model and (b) Force Versus Deflection (y) Response Characteristic of the Rod and c) the Load History (f) Versus Time (t). In (a) the Friction Joint p Slips When the Load Reaches  ${\sf R}_{{\sf m}}$  Representing Plastic Yielding of the Rod

 $\ddot{ }$ 

as the first stage. In this stage, there is no slipping at the joint p. The differential equation of motion and the boundary conditions are:

$$
m\ddot{y} + ky = F_1
$$
 (67)  
 $t = 0, y = 0$  (68)  
 $t = 0, \dot{y} = 0$  (69)

where the differential Equation 67 is based on Newton's second law and the initial conditions state that the initial deflection is equal to the steady downward force of F<sub>1</sub> divided by the spring stiffness and that the initial velocity of the mass is zero. The solution to the differential equation is

 $y = y_{st} + C_1$  Sin wt + C<sub>2</sub> Cos wt

(70)

where  $y_{st} = F_1/k$ . Upon applying the boundary conditions, it is determined .that

 $C_1 = 0$ 

 $C_2 = -y_{st}$ 

(72)

(71)

So the solution can be written as

$$
y = y_{\text{st}} (1-\text{Cos wt})
$$

In Equations 70 and 73,  $\omega$  is the circular frequency defined as

$$
\omega = \sqrt{\frac{k}{m}}
$$
 (74)

The second stage begins at time  $t = t_e$  when the first stage is completed. Time range for the second stage which begins at zero when  $t = t_e$  is established by defining a time variable  $t_i$  for the second stage according to

 $t_i = t - t_e$ 

The differential equation for the second stage is

 $my + R_m = F_1$ 

and the boundary conditions are

 $t_1 = 0$ ,  $y = y_e$ 

 $t_1 = 0$ ,  $y = y_{st} \omega \sin \omega t_e$ 

The general solution to Equation 76 is

(78)

(77)

(75)

(76)

(73)

$$
y = \left(\frac{F_1 - R_m}{2m}\right) t_1^2 + c_1 t_1 + c_2
$$

(79)

Equation 73, which is the dynamic response of the mass during the first stage, can be used to solve for the time  $t<sub>e</sub>$  at which the transition between the two stages occurs:

$$
t_{e} = \frac{1}{\omega} \cos^{-1} \left( 1 - \frac{y_{e}}{y_{st}} \right)
$$
 (80)

Applying the boundary conditions of Equations 77 and 78 to the general solution of Equation 79 gives

$$
y = \frac{1}{2m} (F_1 - R_m) t_1^2 + (y_{st} \omega \sin \omega t_e) t_1 + y_e
$$
 (81)

where  $y_{st} = F_1/k$  is given in Equation 68.

By setting the first derivative of Equation 81 with respect to  $t_1$  to zero, the time at which the displacement of the mass reaches a maximum is found to be

$$
t_1 | y_{\text{max}} = \frac{m y_{\text{st}} \omega \sin \omega t_{\text{e}}}{(R_{\text{m}} - F_1)}
$$

(82)

and the time from the beginning of the transient from Equations 75 and 80 is

$$
t\Big|y_{\max} = \frac{1}{\omega} \cos^{-1} \left(1 - \frac{y_e}{y_{st}}\right) + \frac{my_{st} \omega \sin \omega t_e}{(R_m - F_1)}
$$
(83)

which is more convenient.

Assumptions. In the analysis, it is assumed that the rod material displays linear elastic response followed by perfectly plastic force versus displacement response.

Input Specifications. The problem is completely specified in terms of four parameters  $R_m$ ,  $y_e$ ,  $m$ , and  $F_1$  which allow quantification of k and the other parameters such as w.

- $R_m$  = force necessary to cause yielding in the rod (f) =  $500,000$  (lbf)
- $y_e$  = axial elongation of the rod when plastic deformation begins  $(l) = 0.1666$  (in)
	- k = spring stiffness effort of the rod when deformation is in the elastic range  $(f/l)$  $= R_{m}/y_{e} = 3.0 \times 10^{6}$  (1b/in)
- $m =$  mass attached to the rod  $= 30,000$  (lbf-sec<sup>2</sup>/in)
- $F_1$  = magnitude of uniform tensile force applied to the mass =  $3,000,000$  (lbf)

For these values, Equation 74 gives

 $\omega = 10$  (1/sec)

and Equation 80 gives

 $t_{e} = 0.230$  (sec)

and Equation 82 gives

 $t_1 = 0.1118$  (sec)

so that Equation 75 gives

 $t|_{max} = t_e + t_l$  $t|_{max} = 0.3418$  (sec)

Output Specifications. The output should be the time of maximum deflection of the mass determined by using a structural analysis computer program that will stimulate elastic and plastic material behavior for this structure and its loading.

#### 3.4 Displacement and **Velocity of** Mass When **a** Package **Is Dropped** on a Rigid Floor and the Subsequent Maximum Displacement **of** the Mass and **Maximum Spring** Force

Problem Statement. A mass m represents the contents of a package; the contents are attached to the package with a linear spring of stiffness k. The spring connecting the mass to the package acts in the vertical direction, and all motion of the mass and the package occurs in the vertical direction as shown in Figure 3.4-1.

Objectives. The quantities to be determined are the displacement and velocity of the mass when the container reaches the floor and the subse quent maximum force transmitted to the mass and the required "rattle space" as indicated by the maximum deflection.

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Package System Used to Drop Dynamics Analytical Simulation

Analytical Solution. The dynamics of the package contents are described in Reference TH-65 as

$$
m(\ddot{x}_1 + \ddot{x}_2) + kx_1 = 0
$$

(84)

where

l,

.

m = mass of contents [m]  
\nx<sub>1</sub> = position of the mass relative to the container  
\nmeasured vertically [k]  
\nx<sub>2</sub> = position of container measured vertically [l]  
\nk = linear spring force to displacement ratio [f/l]  
\n
$$
\ddot{x} = \frac{d^2x}{dt^2}
$$
 [l/t<sup>2</sup>]

 $t =$  time measured through the dynamic transient  $[0]$ 

The initial conditions applicable to the first phase of the transient (pre-container impact) are:

 $t = 0, x_1 = 0$ (85)  $t = 0, \dot{x}_1 = 0$ (86)  $t = 0, x_2 = 0$ (87)  $t = 0, x_2 = 0$ 

which state that the initial displacement of~the mass and the container are zero as are their initial velocities in the vertical (downward) direction. All rotation and translation, orthogonal to the vertical, are constrained to zero.

The Laplace transform of the differential Equation 84 for the given initial conditions 2, 3, 4, and 5 is

$$
\bar{x}_{1}(s) = [x_{1}(0) + x_{2}(0)] \frac{s}{s^{2} + \omega_{n}^{2}}
$$
  
+ 
$$
[x_{1}(0) + x_{2}(0)] \frac{1}{s^{2} + \omega_{n}^{2}}
$$
  
- 
$$
\frac{s^{2} \bar{x}_{2}(s)}{s^{2} + \omega_{n}^{2}}
$$

(89)

where

 $\omega_{\bf n}$  =  $\bf v$   $\overline{\bf m}$  = natural frequency of the contents mass,  $\bf m$ , and its attachment spring k to the box [1/e] s = transformed variable replacing time  $[1/\theta]$  $\bar{x}_1(s)$  = Laplace transform of  $x_1(t)$  $\bar{x}_2(s)$  = Laplace transform of  $x_2(t)$ 

The inverse of Equation 89 can be written as

$$
x_{1}(t) = [x_{1}(0) + x_{2}(0)] \cos \omega_{n}t + \frac{1}{\omega_{n}}[\dot{x}_{1}(0) + \dot{x}_{2}(0)] \sin \omega_{n}t
$$
  

$$
-E^{-1} \frac{s^{2} \bar{x}_{2}(s)}{s^{2} + \omega_{n}^{2}}
$$

(90)

The motion of the container is

$$
x_2(t) = \frac{1}{2}gt^2
$$

and its transform is

$$
\bar{x}_2(s) = g/s^3
$$

which when substituted into Equation 89 gives

$$
\bar{x}_1(s) = -\frac{g}{s(s^2 + \omega_n^2)}
$$

for the initial conditions of Equations 85, 86, 87, and 88 and the inverse is

$$
x(t) = -\frac{g}{\omega_n^2} (1 - \cos \omega_n t)
$$

Using Equation 91, the time to fall from the initial height h supporting the container to the floor is

$$
t_o = \sqrt{2h/g}
$$

(95)

(92)

(93)

(94)

The displacement and velocity of the mass m relative to the container when the container impacts the floor are

$$
x_1(t_0) = -\frac{g}{\omega^2} (1-\cos \omega_n t_0)
$$
 (96)

 $x_1(t_0) = -\frac{g}{\omega_n} \sin \omega_n t_0$ (97)

These expressions can be evaluated to give the initial conditions for the second phase of the problem subsequent to the container's impact with the floor.

Redefining a new time variable  $t_1$ , which is zero at the instant the container impacts the floor

$$
t_1 = t - t_0
$$

 $\cdot$ 

(98)

This time variable,  $t_1$ , will be used during the second, post-container impact phase of the problem. The initial conditions for the second phase are

$$
t_1 = 0
$$
,  $x_1 = -g/\omega_n^2$  (1-Cos  $\omega_n t_0$ ) (99)

 $t_1 = 0$ ,  $x_2 = L$ (100)

$$
t_1 = 0, x_1 = g/\omega_n \sin \omega_n t_0
$$
 (101)  
 $t_1 = 0, x_2 = gt_0$  (102)

From Equation 90, the displacement after impact for the initial conditions of Equations 99, 100, 101, and 102 becomes

$$
x_{1}(t) = \left[ n - \frac{g}{\omega_{n}^{2}} (1 - \cos \omega_{n} t_{o}) \right] \cos \omega_{n} t
$$
  
+ 
$$
\frac{1}{\omega_{n}} \left[ g t_{o} - \frac{g}{\omega_{n}} \sin \omega_{n} t_{o} \right] \sin \omega_{n} t
$$
  
- 
$$
h \cos \omega_{n} t
$$

(103)

The first and last terms cancel, and this equation can be rewritten using a trigonometric identity as

$$
x_{1}(t) = \frac{g}{\omega_{n}^{2}} \sqrt{(1-\cos \omega_{n}t_{0})^{2} + [\omega_{n}t_{0} - \sin \omega_{n}t_{0}]^{2}}
$$
  
Sin  $(\omega_{n}t_{1} - \phi)$  (104)

where

where

$$
\phi = \text{Tan}^{-1} \left[ \frac{(1-\cos \omega_n t_o)}{(\omega_n t_o - \sin \omega_n t_o)} \right]
$$

(105)

The maximum amplitude of the mass m is

$$
A = x_1 \Big|_{\text{max}} = \frac{g}{\omega_n^2} \sqrt{(1 - \cos \omega_n t_0)^2 + (\omega_n t_0 - \sin \omega_n t_0)^2}
$$
 (106)

and the maximum occurs at a time consistent with

$$
\omega_n t_1 - \phi = \frac{\pi}{2}
$$
 (107)

or

$$
t_1 = \frac{1}{\omega_n} \left( \frac{\pi}{2} - \phi \right)
$$

(108)

Using Equation 98, the time from the beginning of the first phase of the transient until the maximum displacement of the mass is reached is

$$
t = t_0 + \frac{1}{\omega_n} \left( \frac{\pi}{2} - \phi \right)
$$
 (109)

The maximum spring force is given by

 $F_{max}$  = kA

where

 $k =$  spring stiffness [f/l]

 $A = maximum amplitude of the mass m [2]$ (see Equation 106)

Assumptions.

- The mass m is supported within the box by a linear spring of'stiffness k.
- The mass of the container is large compared to that of the contents, m, so that the free fall of the container is not influenced by the force associated with the relative motion of the mass, m.
- Upon striking the floor, the container remains in contact with the floor.

Input Specifications. For an initial height of the box above the plane of

 $h = 10(in)$ 

the time at which it reaches the plane is given by Equation 95 as

 $t_0$  = 0.2275 (sec)

If the spring stiffness is

 $k = 39.48$  (lb/in)

and the mass of the contents is

 $m = 0.12$  slugs = 3.864 lb<sub>m</sub>

then the circular natural frequency is

$$
\omega_n = \sqrt{\frac{k}{m}} = 20\pi \frac{1}{\sec}
$$

and the vibrational natural frequency is

$$
f_n = \omega_n / 2\pi = 10
$$
 (1/sec)

Equation 106 can be evaluated for

$$
\omega_{\rm n}t_{\rm O} = 20 (0.2275) = 14.29
$$

to give

 $A = 1.306(in)$ 

This is the required rattle space in terms of amplitude.

Output Specifications. The output should simulate the dynamics of this problem with a time history transient analysis program and determine the maximum displacement of the mass after the container strikes the plane and the time at which the maximum amplitude is reached.

## **3.5** Determine **the Natural Frequencies and Normal Modes of** an **Elastic Discrete Mass System**

Problem Statement. This problem concerns the normal modes and natural frequencies of the system shown in Figure 3.5-1, where the two masses each have one translational degree of freedom (in the x direction) and are of equal magnitude as are the three linear spring stiffness values.

Objectives. This analytical solution will provide for numerical testing of all of the frequency extraction and normal mode vector calculation procedures in modal summation type dynamic analysis programs.

Analytical Solution. For the system shown in Figure 3.5-1, the differential equations describing the motion are



Figure 3.5-1

Two Degree of Freedom System for Which the Natural Frequencies and Mode Shapes Will Be Determined

$$
\widetilde{mx}_1 + 2kx_1 - kx_2 = 0
$$

(110)

$$
mx_2 + 2kx_2 - kx_1 = 0
$$

(111)

(112)

(113)

Assume that the motion of each mass is periodic and composed of harmonic motions of various amplitudes and frequencies. Let one of these components be

$$
x_1 = A \sin(\omega t + \phi)
$$

 $x_2 = B \sin (\omega t + \phi)$ 

Substituting Equations 112 and 113 into 110 and 111 gives

$$
(2k-m\omega^2)A-kB=0
$$

(114)

 $-kA + (2k-m\omega^2)B = 0$ 

(115)

which are homogeneous linear algebraic equations for the undetermined  $-magnitudes$  A and B. The trivial solution  $A = B = 0$  is real and represents the static equilibrium position of the masses. The natural frequencies and mode shapes result from

$$
\begin{bmatrix}\n(2k-m\omega^2) & -k \\
-k & (2k-m\omega^2)\n\end{bmatrix}\n\qquad\n\begin{bmatrix}\nA \\
B\n\end{bmatrix}\n=\n\begin{bmatrix}\n0 \\
0 \\
0\n\end{bmatrix}
$$
\n(116)

solving for the values of w which allows the coefficient matrix of Equation 116 to have a determinant equal to zero. The fourth order equation in the circular vibrational frequency of the system is

 $\omega^4$  -  $\frac{4k}{n}$   $\omega^2$  +  $\frac{3k}{2}$ m

(117)

The roots of this equation are



The natural frequencies must be real and positive and are given by Equations 118a and 118b.

By substituting Equation 118a into Equations 114 and 115, the mass displacement amplitude ratio for mode 1 is determined

$$
\frac{A_1}{B_1} = \frac{k}{2k - m\omega_1^2} = \frac{2k - m\omega_1^2}{k}
$$
  

$$
\frac{A_1}{B_1} = 1
$$

(119)

Similarly, by substituting Equation 118b into Equations 114 and 115

$$
\frac{A_2}{B_2} = \frac{k}{2k - m\omega_2^2} = \frac{2k - m\omega_2^2}{k}
$$

(120)

In this way, the amplitude ratios are determined. The mode shapes can't be solved for explicitly but are determined on a relative basis from the amplitude ratios by assuming the displacement amplitude of one of the masses to be unity. Thus, the mode shapes are

 $\begin{bmatrix} A_1 \\ B_1 \end{bmatrix}$  =  $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ 

(121)

.which correspond to the first natural frequency

$$
A_2 = 1
$$

 $B_2 = -1$ 

(122)

which occurs along with the second natural frequency. The mode shapes are drawn in Figure 3.5-2.

Assumptions. It is assumed that the motion of each mass is periodic and composed of harmonic motion of various amplitudes and frequencies. The mode shapes are determined by assuming unit displacement in the positive direction for the mass on the left in Figure 3.5-1.

Input Specifications. The natural frequencies are given by Equations 118a and 118b. For

k = 1.0 lb/in  
\nm = 1.0 lb<sub>m</sub>  
\n
$$
\omega_1 = \sqrt{\frac{\kappa}{m}} = \sqrt{\frac{32.2 (12)}{1}}
$$
\n
$$
\omega_1 = 19.657 (1/sec)
$$
\n
$$
\omega_2 = \sqrt{\frac{3k}{m}} = \sqrt{\frac{3(32.2) (12)}{1}}
$$
\n
$$
\omega_2 = 34.047 (1/sec)
$$



- 2

Figure 3.5-2

Equilibrium Position, Fundamental Frequency and First Mode Shape and Second Natural Frequency and Mode Shape for Two Degree of Freedom Violating System

For  $A_1 = 1.0$ ,  $B_1 = 1.0$  from Equation 119; similarly, from Equation 120 for  $A_2 = 1.0$ , it is determined that  $B_2 = -1.0$ .

Output Specifications. In solving this problem, the dynamics of the mass and elasticity are simulated by a finite element computer model such as ANSYS. The output determines how accurately the model predicts the natural frequencies and mode shapes.

#### **3.6** Determine the **Stress in a Pretensioned Body Which Experiences** Stress **Relaxation** Due **to Creep**

Problem Statement. The ends of a bolt are held a fixed distance apart for a long period of time. Initially, the bolt is tightened producing an initial stress of  $\sigma_0$ . The bolt material is 0.30% carbon steel, which is assumed to have a creep rate given by

 $\int_{E}^{1}C = k$  n

(123)

where

 $\dot{\epsilon}^{\text{C}}$  = creep rate (1/hr)  $k =$  creep constant ( $1/hr$ )  $\sigma$  = axial stress component in bolt (lb/in<sup>2</sup>) n = creep exponent of stress ( )

The creep causes the elastic strain to decrease while the creep strain increases such that the sum of the two is always equal to a constant. The constant is the amount of elastic strain initially induced in the bolt by the initial stress  $\sigma_0$  (see Figure 3.6-1 for a schematic of the bolt).

Objectives. The objective is to calculate the bolt stress as a function of time.



Figure 3.6-1

Bolt of Length 1 in Unloaded State Which Is Inititally Stressed to  $\sigma$  = 10,000 psi and Allowed to Stress Relax Due to Creep

J.

Analytical Solution. It is assumed that the initial stress causes only elastic strain on an instantaneous basis and that the total strain in the bolt remains constant.

$$
\varepsilon_0^e = \varepsilon^e + \varepsilon^c
$$

(124)

where

 $\varepsilon_0^e$  = initial elastic strain ( )  $\varepsilon$ <sup>e</sup> = elastic strain at any time ()  $\varepsilon^C$  = creep strain at any time (initially zero) ()

The elastic strain is related to the stress by Hook's law

$$
\varepsilon_0^e = \frac{\sigma_0}{E}
$$
 (125a)  

$$
\varepsilon^e = \frac{\sigma}{E}
$$

(125b)

**Ii**

where

 $E =$  elastic modulus of bolt material (psi)  $\sigma_0$  = initial axial stress component in bolt (psi)  $\sigma$  = axial stress component in bolt at any time (psi)

Substitution of Equation 125 into Equation 124 gives

$$
\frac{\sigma_0}{E} = \frac{\sigma}{E} + \varepsilon^C
$$

(126)

and the differentiating Equation 126 with respect to time gives

$$
\frac{d\varepsilon^{c}}{dt} = -\frac{1}{E}\frac{d\sigma}{dt}
$$

(127)

where the terms on the left side are the material creep rate. Combining Equations 123 and 127 eliminates the creep rate and gives the first order non-linear differential equation

$$
-\frac{1}{kE} \quad \sigma^{-n} \text{ do } = \text{ dt}
$$

(128)

The initial condition is

$$
t = 0 \qquad \sigma = \sigma
$$

 $(129)$ 

and the solution is of the form

$$
\sigma = \sigma_0 \left[ kE(n-1)\sigma_0^{n-1} t + 1 \right]^{-1/n}
$$

(130)

Assumptions. It is assumed that initially upon loading, the bolt strain is in the elastic range.

Input Specifications. For the following values of the parameters

$$
k = 4.78 \times 10^{-37} (1/hr)
$$
  
n = 6.9 ()  

$$
E = 30 \times 10^{6} (psi)
$$
  

$$
\sigma_0 = 10,000 (psi)
$$

Equation 130 becomes

$$
\sigma = 10,000 \left[3.368 \times 10^{-5} \text{ t} + 1\right]^{-0.1695}
$$

(131)

which can be evaluated to give:



Output Specifications. The output indicates the stress in the bolt as a function of time using the creep strain features of a finite element analysis program.

## 3.7 Elastic Stability of a Thin Tube of Infinite Length with External Pressure Loading

Problem Statement. The solution of this problem determines the magnitude of the external pressure loading that will cause a long, thin-walled, cylindrical tube to reach elastic instability. The cylinder configuration and pressure loading are shown in Figure 3.7-1.

Objectives. This problem will test the elastic stability prediction capability of structural analysis programs.

Analytical Solution. The solution given by Roary (Reference RO-65) for the external pressure load limit based on elastic stability is

$$
p = \frac{1}{4} \frac{E}{1-v^2} (\frac{t}{r})^3
$$

(132)

where

 $p =$  limit external pressure load [f/ $\ell^2$ ] E = elastic modules of tube material  $[f/g^2]$  $v = Poisson's ratio of tube material$  [ ]  $t =$  tube wall thickness  $[\ell]$  $r =$  tube radius  $\lceil \ell \rceil$ 

The buckling solution should apply providing that the structure does not fail due to yielding (see Figure 3.7-2). According to the Tresca criterion, yielding will not occur providing that

$$
\sigma_i < \sigma_t = \frac{pr}{t} < \sigma_{cy}
$$

(133)



# Figure **3.7-1**

Long, Thin-Walled Circular Cylinder Loaded with lled Circular Cyl





Compressive Yield and Buckling Failure Required for a Long Cylinder. External Pressure Is Plotted Against Cylinder Geometric Feature **(r/t)** where\*

 $\sigma_i$  = Tresca stress intensity [f/ $l^2$ ]  $\sigma_t$  = compressive hoop stress component  $\sigma_{CV}$  = material yield stress in compression  $[f/\ell^2]$ *[fi* 2]

Equation 132 can be rewritten in terms of the hoop stress  $\sigma_t$  at which the cylinder becomes elastically unstable  $\sigma_{EU}$  as

$$
\sigma_{EU} = \frac{1}{4} \frac{E}{1-v^2} (t_r)^2
$$

(134)

The tube should then have a stress  $\sigma_t$  such that  $\sigma_t < \sigma_{EU}$  and  $\sigma_t < \sigma_{Cy}$ . The limiting pressure becomes

$$
p = min
$$
  $\begin{cases} \sigma_{cy} (t/r) = p_{cy} \\ \frac{1}{4} \frac{E}{1-v^2} (t/r)^3 = p_{EU} \end{cases}$ 

(135)

based on Equations 133 and 132 with  $\sigma_t = \sigma_{cy}$ . To obtain buckling failure

$$
P_{EU} < P_{cy}
$$

(136)

\*In this problem, it is convenient to consider compressive stresses and the compressive yield stress  $\sigma_{CY}$  as positive quantities. This sign convention will apply to this problem.

from Equation 135. Substituting Equation 135 into Equation 136 gives

$$
\frac{r}{t} > \sqrt{\frac{E}{4(1-v^2) \sigma_{cy}}} = \left(\frac{r}{t}\right)_{ref}
$$

(137)

to assure buckling failure. Thus, when r/t > (r/t)<sub>ref</sub>, buckling failure is expected, and when r/t < (r/t)<sub>ref</sub>, compressive yield failure is expected.

If  $E = 3 \times 10^6$  (psi) and  $v = 0.3$  as is typical for some steels, the  $(r/t)_{ref}$  for various values of  $\sigma_{cy}$  is given in Table 3.7-1.

Assumptions. It is assumed that the cylinder is round and of uniform thickness and that the deformed shape is oval. The material properties are assumed to be isotropic.

Input Specifications. The following material properties must be defined:

• Elastic modulus =  $E = 30 \times 10^6$  (psi)

• Poisson's ratio =  $v = 0.30$  ()

- Compressive yield strength =  $\sigma_{CV}$  = 30,000 (psi)
- Cylindrical tube mean radius =  $r = 20$  (in)
- Cylindrical tube wall thickness =  $t = 1$  (in)

The external pressure loading that will cause buckling is determined . by

 $r/t = 20$ 

# Table 3.7-1

 $\mathcal{E}$ 

Values of (r/t)<sub>ref</sub> at Which Failure Mode Changes Versus Compressive Yield Strength,  $\sigma_{\text{Cy}}$ , for Steel Type Materials Where E=30x10<sup>6</sup> and  $v=0.3$ 


and for  $\sigma_{cy}$  = 30,000 psi;  $(r/t)_{ref}$  = 16.6. Since r/t >  $(r/t)_{ref}$ , buckling failure should occur.

For this case, Equations 132 and 134 give

p = 1030 (psi)

 $\sigma_{\text{FII}}$  = 20,600 (psi)

and the latter is clearly less than the  $\sigma_{CV}$ . Equation 133 allows a 1500 psi pressure because buckling is more limiting when  $r/t > (r/t)_{ref}$ .

Output Specifications. The output should include:

- Dimensions
- Material properties
- Allowable external pressure based on elastic instability (check against Equation 132 value)
- Elastic instability hoop stress  $\sigma_{\text{FI}}$  (check against Equation 134 value)

#### 3.8 Creep Deformation of a Finite Length, Hollow Elastic Cylinder Due to External Pressure

Problem Statement. A hollow cylinder of finite length is subjected to external pressure loading (see Figure 3.8-1). The pressure acts both radially and axially.

Objectives. The objective of this problem is to compare the COVE program's creep deformation predictions with analytical and experimental observations. Typically, poor agreement is achieved between analytical predictions of collapse and experiments. A specific objective is to determine whether COVE results are conservative relative to experimental determinations of when collapse occurs.



**P= 2700 (psi) (for 100 hr.)**

 $r_m = 0.1285$  (in)

 $t = 0.012$  (in)

 $T = 680 (°F)$ 

Figure 3.8-1.

Finite Length Hollow cylinder Subjected to External Pressure Loading

Analytical Solution. Griffin (GR-67) has proposed a simplified theory of creep collapse which is analogous to instantaneous elastic-inelastic creep collapse. It uses isochronous stress strain curves instead of instantaneous stress strain curves. The isochronous stress-strain curves give the stress as a function of strain after having the load applied for a fixed time.

The collapse is predicted using

 $\sigma_{\rho}$  = -pr/t (138)  $\sigma_x = -\frac{pr}{2t}$  $\sim 10^{-11}$ (139)  $\tau_{\chi\theta} = 0$ (140)

-The von Mises stress intensity for these stress components is

 $\sigma_i = \frac{\sqrt{3}}{2}$  Pr

(141)

The critical or buckling stress is calculated from

$$
\sigma_{\theta}|_{b} = \frac{nE_{s} t^{2}}{4(1-v^{2}) r^{2}}
$$

 $\ddotsc$ 

(142)

$$
\eta = 1 - \frac{(1 - E_t/E_s)}{1 + (1 - 4v^2) Et/3E_s}
$$



where

- **i** = correction factor which takes into account nonlinear nature of the isochronous stress-strain curve [ ]
- $E_t$  = tangent of the isochronous stress-strain curve at the point describing the state of stress  $\sigma_i$  [psi]
- $E_S$  = ratio of stress to strain at the point describing<br>the state of stress  $\sigma_i$  [psi] the state of stress  $\sigma$
- $v = Poisson's ratio of the material$  [ ]
- $t = cylinder$  radial wall thickness [in]
- $r =$  mean radius of the cylinder wall  $[in]$
- $\sigma_{\theta}$  = value of hoop stress at which buckling is predicted<br>b to occur [psi] to occur

In Equations 142 and 143, the moduli  $E_t$  and  $E_s$  correspond to a state of stress as represented by the von Mises stress intensity given by Equation 141.

Figure 3.8-2 gives the generalized stress versus strain curve for various values of the Larson-Miller parameter (LMP) given by

LMP =  $(T + 460)$  (20 + log<sub>10</sub>  $\tau$ )

(144)

where



**Figure 3.8-2**

Iso-LMP Stress-Strain Curves for **15X** Cold Worked **Zircaloy in the** . 550 to 750°F Temperature Range

 $T =$  temperature of material  $[OF]$ 

-

- = duration of loading (hrs]
- LMP = combined time and temperature parameter used in correlating creep strain effects [ ]

These curves shown in Figure 3.8-2 are used as isochronous stress-strain curves.

Assumptions. In the analysis, the cylinder is assumed to have an initial ovality which is typical of the tolerance on roundness as described by diametral dimensions:

$$
U = U_0 \cos 2\theta
$$

Input Specifications. For 15% cold-worked Zircaloy tubing material, the following conditions define the geometry of the cylinder, its loading and the atmospheric conditions:

 $p =$  external pressure = 2700 (psi)

 $T = material temperature = 680 (OF)$ 

 $t = cyline$  wall thickness = 0.013 (in)

 $U<sub>O</sub>$  = initial ovality = .0005

 $r = cyline$  mean radius = 0.1285 (in)

LMP = Larson-Miller parameter (from Equation 144) =  $23,940$  ()

 $L =$  tube length = 144 (in)

 $v = Poisson's ratio = 0.25$  ( )

 $E_t$  = tangent modulus (see Figure 3.8-2 for values) [psi]

 $E_S$  = secant modulus (see Figure 3.8-2 for values) [psi] ]

Griffin (Reference GR-67) has analyzed this case using Equations 142 and 143 along with Figure 3.8-2. Collapse in less than 10 hours was predicted. He also reports limited test data in which collapse occurred before the first observation, which was made after 72 hours of loading.

Output Specifications. The output indicates whether substantial magnification of ovality approaching the equivalent of collapse is predicted with the COVE program to have occurred within 10 hours. If it is predicted, this would be an indication that COVE is likely to be conservative.

Collapse often depends on individual properties of specimens and loading conditions beyond those described by average properties. Analytical prediction methods are generally not very precise.

### 3.9 Hypothetical Prediction of Deformation Including Progressive Creep for a Waste Package

Problem Statement. The waste package must function for a very long time. External loads due to groundwater pressure or rock forces could act during most or all of the waste package service life. The cumulative effects of these loads of long duration are much greater than the effects of shorter duration. Therefore, creep strain must be considered because its contribution to total strain may be much greater than the instantaneous strain. Creep strain causes additional ductility to be consumed which must be accounted for in the structural integrity assessment.

This problem considers a long cylindrical overpack reinforcement as shown in Figure 3.9-1. The waste package is proportioned so that the reinforcement is relied on to resist the entire external load.

Objectives. The objectives of this analysis are

- To demonstrate a method for estimating creep strain in a waste package structure
- . To estimate the creep strains for a particular waste package





Hollow Cylindrical Overpack Reinforcement Structure for a Waste Package cal Overpack Reinforcement Structure 1

 $\hat{\mathcal{A}}$ 

Analytical Solution. This is a hypothetical problem. An analytical solution will not be presented for comparison with the computer program solution.

Assumptions. In posing the problem, it is assumed that the overpack reinforcement carries all of the externally applied structural load. This is consistent with the assumptions made during the conceptual design process for waste packages to be emplaced in tuff.

It will be assumed that the carbon steel maintains a secondary creep rate during the entire loading duration.

Input Specifications. The configuration for the waste package (Reference ON-83, p. 15) is:

$$
D_0 = 55
$$
 (cm)  
 $t = 2.5$  (cm)  
 $\ell = 4.1$  (m)

The loading is a uniform external pressure on the cylinder

$$
p = 2250 (psi)
$$
  
t = duration of loading = 1,000 (years)  
T = 400 (OC)

The creep rate is taken to be of the form

$$
\epsilon^c \frac{d\epsilon^c}{dt} = k\sigma^n
$$

where

 $k = 48 \times 10^{-38}$  [1/hr]  $n = 6.9$  []

(145)

giving a creep strain rate of

$$
\dot{\epsilon}^{\text{C}_{\text{m}}} = 9.93 \times 10^{-7} \left[ \frac{1}{\text{hr}} \right]
$$

for the stress of

$$
\sigma = \frac{pr}{t} = 2250 (55/2) (1/2.5)
$$
  

$$
\sigma = 24,750 [psi]
$$

The overpack and overpack reinforcement are fabricated from carbon steel. The material properties are

 $E =$  elastic modulus = 27.4 x 10<sup>6</sup> (psi)  $v = Poisson's ratio = 0.30$  ()

Output Specifications. The solution compares the creep strain and the ratio of total strain to instantaneous strain and the ratio of creep strain to instantaneous strain after several loading intervals such as 10, 100, 300, and 1,000 years.

#### 3.10 Hypothetical Calculation of Stress Resulting **from a** Steady-State Temperature Distribution in a Waste Package

Problem Statement. This problem is designed to determine the hoop stress component distribution in a series of n concentric hollow cylinders (annular sections). The stress distribution is the result of a radial temperature distribution in the hollow cylinders.

The n concentric hollow cylinders (annular sections) surround a solid cylinder acted on by a spatially uniform heat generation representative of the waste acts. The concentric hollow cylinders each have a predetermined temperature distribution. This results from the solution of Problem 2.5. The purpose of this problem is to impose those temperatures along with sufficient mechanical properties so the state of stress can be determined at the inside and outside radius of each of the annuli. The concentric cylinders are shown in Figure 3.10-1.

Objectives. This problem is useful in representing a waste package region such as a thick self-shielding canister. The annular regions are arbitrarily defined in that they are subregions of a larger continuous wall of the canister. Because different physical properties are present in the different regions, it is not convenient to obtain an analytical solution. Solution comparisons between WAPPA and ANSYS are intended.

Analytical Solution. This problem does not have an analytical solution that can be readily obtained (without the linear equations solution capabilities of structural programs). Modeling will be done on as nearly an equivalent basis as possible with the WAPPA and ANSYS programs, and the resulting solution **in** terms of stress values will be compared.

Assumptions. It is assumed that the mechanical properties are uniform and constant in each region.

Input Specifications (see Reference ON-83). The radial temperature distribution will be as determined in the solution to Problem 2.5.

Geometry (See Figure 3.10-1) - radii  $r_0^7$  = 65 (cm)  $r_0^6 = r_1^3 = 60$  (cm)  $r_05 = r_16 = 55$  (cm)

139



# Figure 3.10-1

n Concentric Cylindrical Annuli with Known Outside Temperature T<sub>O</sub>, Surrounding a Waste Region of Radius r<sub>w</sub> in Which a Known Volumetric Heat Generation Rate q''' Exists. Each Region Can Have Its Unique Set of Mechanical Properties

$$
r_0^4 = r_1^5 = 50 \text{ (cm)}
$$
  
\n
$$
r_0^3 = r_1^4 = 45 \text{ (cm)}
$$
  
\n
$$
r_0^2 = r_1^3 = 40 \text{ (cm)}
$$
  
\n
$$
r_0^1 = r_1^2 = 35 \text{ (cm)}
$$
  
\n
$$
r_1^1 = r_0^w = 30.5 \text{ (cm)}
$$
  
\n
$$
r_1^w = 0
$$

# Material Properties.

\n- Elastic modulus\n 
$$
E^7 = 27.4 \times 10^6
$$
 (psi)\n  $E^6 = 27.0 \times 10^6$  (psi)\n  $E^5 = 26.6 \times 10^6$  (psi)\n  $E^4 = 26.2 \times 10^6$  (psi)\n  $E^3 = 25.8 \times 10^6$  (psi)\n  $E^1 = 25.0 \times 10^6$  (psi)\n  $E^N = 10.0 \times 10^6$  (psi)\n  $E^N = 10.0 \times 10^6$  (psi)\n  $V^7 = 0.30$ \n $V^7 = 0.30$ \n $V^6 = 0.30$ \n $V^4 = 0.30$ \n $V^2 = 0.20$ \n
\n

Temperature coefficient of thermal expansion

 $\alpha$ <sup>7</sup> = 6.52 x 10<sup>-6</sup> (1/<sup>o</sup>F)  $\alpha$ <sup>6</sup> = 6.55 x 10<sup>-6</sup> (1/<sup>o</sup>F)  $\alpha^{5}$  = 6.58 x 10-6 (1/OF)  $\alpha$ <sup>4</sup> = 6.61 x 10<sup>-6</sup> (1/<sup>o</sup>F)  $\alpha^3$  = 6.64 x 10<sup>-6</sup> (1/<sup>O</sup>F)  $\alpha^2$  = 6.67 x 10-6 (1/OF)  $\alpha$ <sup>1</sup> = 6.70 x 10<sup>-6</sup> (1/<sup>o</sup>F)  $\alpha^{W}$  = 6.78 x 10<sup>-6</sup> (1/<sup>O</sup>F)

Output Specifications. The output will be the stresses at the inside and outside radii of each of the annular sections which make up the waste package.

### 3.11 Hypothetical Analyses of Canister Stresses Subsequent to Being Filled with a Hot Glass Waste Form

Problem Statement. Some thermal conditions produce large internal forces and moments and hence stress values because different portions of the structure are at different temperatures. Since these different portions of the structure are connected, they constrain each other from the independent, free expansion necessary to receive internal forces, moments, and thermal stresses. The performance assessment of canisters into which molten glass waste forms are poured should be analyzed to determine the stress values resulting from the temperature distribution which exists at various times subsequent to filling. The temperature distributions are determined in Problem 2.7. Figure 3.11-1 shows the canister before filling.

Objectives. The objective of this problem is to solve for the structural response caused by severe temperature gradients in a canister. The

142





Canister into Which Molten Glass Waste Is Poured

quantities of interest will be the stress values throughout the structure. The known temperature distributions at various times in the transient will be the loading conditions.

Analytical Solution. This is a hypothetical problem. A computer program model will be developed and structural response simulated. It is anticipated that the ANSYS computer program will be used. An independent analytical solution will not be determined.

Assumptions. It is assumed that the molten waste form is poured instantaneously into the canister at time zero.

-Input Specifications. The structural analysis will be for the configuration and heat transfer conditions given in Table 3.11-1. The mechanical properties (in English units) as a function of temperature for 304 stainless steel are



#### Legend

- E Elastic Modulus
- v Poisson's Ratio
- G Shear Modulus (Lame's Constant  $\mu$ )
- $\lambda$  Lame's Constant
- K Bulk Modulus
- $\alpha$  Mean Coefficient of Thermal Expansion from 700F to the Indicated Temperature

# Table 3.11-1

 $\bullet$ 

l,

 $\ddot{\phantom{a}}$ 

 $\ddot{\phantom{a}}$ 

÷,

 $\hat{\mathcal{A}}$ 

 $\overline{a}$ 

In Development

 $\overline{a}$ 

Similarly, the glass mechanical properties (in metric units) are:



#### Legend

E - Elastic Modulus  $v -$  Poisson's Ratio G - Shear Modulus (Lame's Constant  $\mu$ )  $\lambda$  - Lame's Constant K - Bulk Modulus  $\alpha$  - Coefficient of Thermal Expansion

Output Specifications. Generalized stress intensity values will be monitored at various node locations throughout the canister wall thickness and examined for reasonableness.

### 3.12 Hypothetical Calculation of Stress Due to Uniform External Pressures on a Waste Package

Problem Statement. A waste package structure is loaded by uniform external pressure. Only instantaneous structural response to the loading is to be considered. Material deformation is in the elastic range. The loading is substantial but not large enough to cause instantaneous plastic deformation.

A sketch of the structure is shown in Figure 3.12-1. The inside and outside radius of the structure's cylindrical annulus cross section are denoted by  $r_i$  and  $r_0$ . Intermediate positions are denoted by  $r_a$ ,  $r_b$ , and  $r_c$  as shown in Figure 3.12-1.

Objectives. The objectives of this problem are to compare structural responses predicted by WAPPA to those obtained from a finite element program. The ANSYS finite element program will be used to generate

146



Figure 3.12-1

Waste Package Structure with Uniform External Pressure Loading

comparative responses. Stress components in the tangential direction at various radial positions will be the principal quantity of interest.

Analytical Solution. This is a hypothetical problem in which WAPPA and ANSYS are to be compared. The thick-walled cylinder solution for the stress component in the circumferential direction as a function of radial position, inside and outside radius, and external pressure can readily be used to obtain an additional check. The tangential stress component is given by

$$
\sigma_t = -\frac{p_0 r_0^2}{r_0^2 - r_i^2} \quad (1 + \frac{r_i^2}{r^2})
$$

-

$$
(146)
$$

where

 $p_0$  = uniform external pressure acting at radius  $r_0$  [f/ $\ell^2$ ]

 $r_0$  = outside radius  $\lbrack l \rbrack$ 

 $r_i$  = inside radius  $[2]$ 

r = particular position of interest in the range  $r_i \leq r \leq r_0$  [2]

 $\sigma_t$  = tangential stress quantity at radius r [f/ $\ell^2$ ]

Assumptions. It is assumed that pressure is not applied to the ends of the cylinder.

Input Specifications. A static pressure loading of 5 MPa will be applied to the following carbon steel overpack structure:

Outside radius =  $r_0$  = 32.25 (cm) Inside radius =  $r_i$  = 29.75 (cm)

The intermediate radial positions are at:

r<sub>a</sub> = 30.375 (cm r<sub>b</sub> = 31.000 (cm r $_{\rm C}$  = 31.625 (cm

Output Specifications. The tangential stress component at radii ri, ra,  $r_b$ ,  $r_c$ , and  $r_0$  are to be evaluated. Using Equation 146 for the given pressure loading and annular dimensions, the tangential stress component is predicted to be:



#### 4.0 RADIATION SHIELDING PROBLEMS

This section deals with the shielding of neutrons and gamma rays within the waste form and the surrounding waste canister. It contains five problems:

- A simple problem to allow comparison of the "buildup factor" method with more sophisticated transport theory shielding codes
- Measured radiation fields around a PWR fuel assembly in air and water
- Measured radiation levels around a BWR fuel assembly in air and water
- A hypothetical shielding problem for a thick-walled waste package
- A hypothetical shielding problem for a thin-walled waste package

These problems can be used to aid in verifying and validating radiation shielding codes.

### 4.1 Hypothetical Radiation Shielding Problem

Problem Statement. The problem requires the estimation of the gamma flux and dose at the outer surface of a concrete drum containing a 1 MeV gamma source. Three subproblems are presented: no external shield, a 5 cm steel shield, and a 25 cm steel shield. This is a relatively simple problem that can be solved analytically by the buildup factor method.

Objectives. The purpose of this problem is to compare the predictive capabilities of a simple analytical shielding calculation and a transport theory computer code calculation.

Physical Description. A long concrete cylinder contains a uniformly dispersed 1 MeV gamma emitter with a source strength of  $10<sup>7</sup>$  disintegrations

150

per cubic centimeter per second. The cylinder is 0.60 m in diameter and, for purposes of the analysis, is assumed to be infinitely long. The gamma flux and dose rate are to be calculated for a bare cylinder and for cylinders with 5 cm and 25 cm annular steel shields.

Analytical Solution. This problem can be solved analytically using methods described in Reference RO-56. This method assumes that the shield is a slab. This is a good approximation for the 5 cm thick shield but may be a poor assumption for the 25 cm shield.

For an infinite length cylindrical source, the gamma flux,  $\phi$ , at an exterior point is given by:

$$
\phi = \frac{BS_{\nu}R_{0}^{2}}{2(a+z)} \quad F(\frac{\pi}{2},b_{2})
$$

(147)

where:

 $\phi$  = gamma flux, photons/cm<sup>2</sup>-sec B = buildup factor, dimensionless  $S_V$  = volumetric photon source, photons/cm<sup>3</sup>·sec  $R_0$  = radius of cylinder, cm a = distance from cylinder surface to measurement point, cm  $z =$  effective source self-attenuation distance, cm **π/2** (F½,b<sub>2</sub>)= J<sub>o</sub> e-b2 secθ<sub>dθ</sub>, Sieverts integral or secant integral, dimensionless

The buildup factor, B, is defined as the rate of the actual gamma flux compared to that calculated using exponential attenuation with the linear attenuation coefficient. Table 4.1-1 gives dose buildup factors and attenuation coefficients for 1 MeV gamma photons in selected materials.

The effective source self-attenuation distance can be calculated using figures in Reference RO-56. The calculated values of z as a function of shield thickness are given below:



Buildup factors in concrete and iron calculated using values from Table 4.1-1 are given in Table 4.1-2. The total number of relaxation lengths (b2) can be calculated from the equation:

 $b_2 = u_c z + \mu_1 t$ 

where:

 $\mu_c$  = the gamma absorption coefficient for concrete  $H_1$  = the gamma absorption coefficient for iron t = the thickness of the iron shield

Calculated values of b<sub>2</sub> are given below:



The calculated values of b<sub>2</sub> are used to determine  $F(\pi/2,b_2)$  from figures in Reference RO-56.





### Dose Buildup Factors and Attenuation Coefficients for 1 MeV Gama Rays

 $B(\mu_t x) = A_1 \exp (-\alpha_1 x) + (1-A_1) \exp (-\alpha_2 x)$ Dose =  $E\phi(E)\mu_e/\rho$  MeV/cm<sup>3</sup>.sec =  $5.767 \times 10^{-5}$  E $\phi$  (E) $\mu$ <sub>e</sub>/p Rad/hr \*

\* 5.767 x 10<sup>-5</sup> = 
$$
\frac{1.602 \times 10^{-6} \text{ erg}}{M \text{eV}}
$$
  $\frac{1 \text{ Rad}}{100 \text{ erg/g}}$   $\frac{1}{\rho} \frac{1}{g/cm^3}$   $\frac{3600g}{hr}$ 

Source: AN-63

# Table  $4.1-2$

# Calculated Buildup Factors

# No Shield

 $\text{Borel}$ 

$$
B_C = 10 \exp(.088 \cdot .1492 \cdot 25.8) - 9 \exp(-.029 \cdot .1492 \cdot 25.8)
$$
  
= 6.1

 $\mathbf{p} = \mathbf{p} \mathbf{p} \mathbf{p}$ 

$$
B_1 = 8 \, \text{exp} \, (.0895 \cdot .4677 \cdot 0) - 7 \, \text{exp} \, (-.04 \cdot .4677 \cdot 0)
$$

$$
B_{\text{system}} = B_{\text{c}} \cdot B_{\text{I}}
$$

# 5 cm Shield

Concrete experiment in the contract of the contract of

$$
B_C = 10 \exp (.088 \cdot .1492 \cdot 26.4) - 9 \exp (-.029 \cdot .1492 \cdot 26.4)
$$
  
= 6.1

 $\mathbf{F}$  $=$  3.5  $\pm$  3

$$
B_1 = 8 \exp (.0895 \cdot .4677 \cdot 5) - 7 \exp (-.04 \cdot .4677 \cdot 5)
$$
  
= 3.5  

$$
B_{\text{system}} = B_{\text{c}} \cdot B_1
$$
  
= 6.1.3.5  
= 21.4

Concrete

$$
B_C \approx 10 \exp(.088 \cdot .1492 \cdot 23.5) - 9 \exp(-.029 \cdot .1492 \cdot 23.5)
$$
  
= 5.6

 $\ddot{\phantom{a}}$ 

 $\mathbf{F}_{\mathbf{R}}$  $\blacksquare$ 

 $\bar{z}$ 

$$
B_1 = 8 \, \text{exp} \, (.0895 \cdot .4677 \cdot 25) - 7 \, \text{exp} \, (-.04 \cdot .4677 \cdot 25) \\ = 18.0
$$

 $B<sub>cycle</sub>$ 

# **Table 4.1-2**

# Calculated Buildup Factors

# No Shield

Concrete

$$
B_C = 10 \exp (.088 \cdot .1492 \cdot 25.8) - 9 \exp(-.029 \cdot .1492 \cdot 25.8)
$$
  
= 6.1

 $\sim$ 

Iron

$$
B_1 = 8 \, \text{exp} \, (0.0895 \cdot 0.4677 \cdot 0) - 7(-0.04 \cdot 0.4677 \cdot 0) = 1
$$

$$
B_{system} = B_{c} \cdot B_{I}
$$

$$
= 6.1
$$

5 cm Shield

Concrete

$$
B_{C} = 10 \exp (.088 \cdot .1492 \cdot 26.4) - 9 \exp (-.029 \cdot .1492 \cdot 26.4)
$$
  
= 6.1

Iron

$$
BI = 8 exp (.0895 \cdot .4677 \cdot 5) - 7 exp (-.04 \cdot .4677 \cdot 5)
$$
  
= 3.5  

$$
Bsystem = BC \cdot BI
$$
  
= 6.1 \cdot 3.5  
= 21.4

25 cm Shield

Concrete

$$
B_{C} = 10 \exp (.088 \cdot .1492 \cdot 23.5) - 9 \exp (-.029 \cdot .1492 \cdot 23.5)
$$
  
= 5.6

Iron

$$
B_{I} = 8 \exp (.0895 \cdot .4677 \cdot 25) - 7 \exp (-.04 \cdot .4677 \cdot 25)
$$
  
= 18.0  

$$
B_{system} = B_{C} \cdot B_{I}
$$
  
= 5.6.18  
= 101.4



Substituting these values into the equation for the flux and dose at the center surface, the following are obtained:



Assumptions. The concrete isotopic content in Table 4.1-3 should be used to estimate the gamma flux using a transport theory code.

Output Specifications. The outputs for this problem are the gamma photon flux and the dose rate at the outer shield surface.

Comments. The results given here should be compared with the results from a one-dimensional transport theory calculation and the shielding factor method employed in the codes BARIER and WAPPA. For the 0 cm and 5 cm shields, good agreement  $(20\%)$  between the results given here and code predictions can be expected. For the 25 cm shield, the results predicted in this report may vary from predictions derived from a transport theory code because of the difficulty in calculating attenuation in thick shields using the shielding factor method.

4.2 Pressurized Water Reactor Fuel Assembly Radiation Levels

Problem Statement. This problem presents the results of in-plant test measurements of the radiation field in air and water around a Pressurized Water Reactor (PWR) fuel assembly from Point Beach Unit 2. The problem is based on measurements taken at General Electric's Morris Operation.

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### **Table 4.1-3**

Elemental Content of Type 04 Cement\*



Source: AN-63, p. 660. Na content corrected from 0.400 to 0.040. Water content increased slightly (H from 0.013 to 0.014, 0 from 0.103 to 0.111) to agree with density of 2.35 g/cm3.

Objectives. This problem will provide a basis for comparing the radiation field calculated using a source term code and a shielding code with measured experimental data.

Physical Description. Point Beach Unit 2 uses Westinghouse 14x14 fuel assemblies. The fuel was irradiated from August 1972 to March 1977. After discharge from the reactor and cooling, the fuel was shipped to General Electric's Morris Operation for interim storage. As part of an engineering and test support contract funded by the Department of Energy, selected fuel assemblies were characterized. Gamma exposure rates near spent fuel assemblies were measured four years after discharge of the fuel from the reactor.

Fuel assembly design characteristics are given in Table 4.2-1. The initial non-actinide composition of uranium oxide fuel pellets is given in Table 4.2-2. The weight of fuel assembly structural materials is presented in Table 4.2-3, and the elemental composition of structural material is given in Table 4.2-4. Fuel assembly operating conditions are summarized in Table 4.2-5.

The concentrations of fuel assembly structural material located in the end fitting zone should be multiplied by 0.011 to account for the lower activation levels near the ends of the fuel assembly due to flux levels lower than those in the active fuel zone. In addition, the concentrations of manganese, cobalt, and zirconium in the end fitting zone should be multiplied by factors of 0.80, 0.67, and 0.40, respectively. These corrections account for the difference between the neutron energy spectrum in that zone and the spectrum in the active fuel zone. Both kinds of corrections are based on axial spectrum calculations for a Westinghouse PWR fuel assembly as reported in Reference CR-78. With these corrections, the ORIGEN-S calculations should more accurately predict the nuclide activities from the structural materials.

Reference JU-81 gives the results of experimental measurement of gamma dose rate and calculations using the shielding factor code QAD. These

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### **Table 4.2-1**

Fuel Design Data for Point Beach 2



a Theoretical U02 density is 10.96 g cm-3.

b VF is a SAS2 parameter related to volume fraction and/or percent theoretical density (see Reference OR-82).

# Table **4.2-2**



Typical Non-actinide (Impurity) Composition of LWR Oxide Fuels

### Source: MI-83

 $\ddot{\phantom{a}}$ 

a Parts of element per million parts of heavy metal.



Typical PWR Fuel Assembly Structural Material Mass Distribution



Source: MI-83

i

a Distribution throughout the PWR core in sleeves and so forth.



 $\sim 10$ 

 $\bar{\mathbf{v}}$ 

 $\Delta$ 

Typical Elemental Compositions of LWR Fuel Assembly Structural Materials



Source: MI-83

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 $\sim$ 

<sup>a</sup> Value used in source term calculations should are not in the active fuel zone. be less than this (actual) value if the materials

### Table 4.2-5



### Fuel Assembly Operating Conditions

In Development

\* After initial startup, the plant operated at 20% power for seven months due to operating license restrictions.

Source:

results are given for measurements taken at several axial locations for the X-Y detector location given in Table 4.2-6. Table 4.2-7 gives the calculated intensities for the gamma radiation source in spent fuel from Reference JU-81.

Table 4.2-8 gives the measured gamma exposure rates at the fuel assembly mid-point along the "Bl" profile for three fuel assemblies that were believed to have similar irradiation histories. In addition to measured exposures at each corner, Table 4.2-8 provides an indication of the anisotropy of gamma exposure. For individual fuel assemblies, the measured gamma exposure varied by as much as  $\pm 8\%$ . (In calculating the gamma intensity around a fuel assembly, it is commonly assumed that the fuel burnup and therefore the gamma source is evenly distributed.)

Results of additional measurements made along the Bl profile at 1 ft intervals are given in Table 4.2-9. These measurements provide an estimate of the standard error of the exposure rate measurement of about  $\pm 4\%$ (one sigma).

Table 4.2-10 gives results of calculated and measured exposure rates in air and water for three detector profiles.

Reference JU-81 includes a discussion of the accuracy and precision of measured results. Based on an analysis of all identified sources of random errors, the overall variability of measurement is estimated to be 3.8%. This reference also states that based on measurements performed by GE, a variance of  $\pm 3\%$  (one sigma) between utility-calculated fuel exposures and true exposures may exist. This agrees with generally held beliefs about the accuracy of these calculations and is consistent with IAEA guidelines established for safeguards purposes.

Assumptions. Analyses may be performed using the following assumptions:

The entire fuel assembly (except end fittings) is a homogeneous mass.

The two outer rows of fuel rods are modeled discretely; the remaining rods are a homogeneous mass.
l Gamma Detector Locations



 $\stackrel{\text{\tiny{*}}}{\text{\tiny{*}}}$  The origin is the corner of the fuel assembly envelope at the top of the active length of the fuel.

\*\* This detector is located above the fuel assembly.

#### Calculated Gamma Intensities for Gamma Radiation Sources in Spent Fuel



### Source: JU-81

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 $\overline{a}$ 

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 $\ddot{\phantom{0}}$ 

## Exposure Rates from Fuel Assemblies



 $\omega_{\rm s}$ 

Source: JU-81

 $\Delta \sim 10$ 

 $\Delta \phi$ 

 $\sim 10^{-5}$ 

 $\sim$ 

 $\sim 10^{11}$  km  $^{-1}$ 

 $\bullet$ 

 $\langle \mathbf{v} \rangle$ 

 $\sim 10^7$ 

### Exposure Rate from Repeated Fuel Assembly Measurements



\* Distance from the top of the active fuel height.

Source: JU-81

 $\mathcal{L}^{\text{max}}_{\text{max}}$  , where  $\mathcal{L}^{\text{max}}_{\text{max}}$ 

 $\sim 10^7$ 

 $\mathcal{L}$ 

 $\mathcal{L}^{\mathcal{L}}(\mathcal{L}^{\mathcal{L}}(\mathcal{L}^{\mathcal{L}}(\mathcal{L}^{\mathcal{L}})))$ 

 $\sim$ 

 $\sim 100$ 

 $\mathcal{A}^{\pm}$ 



## Calculated and Measured Exposure Rates

\*Feet below top of fuel assembly active height.

Source: JU-81

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 $\lambda$ 

#### Additional simplifying assumptions are:

- Spacer grids are homogenized over the entire assembly.
- Fuel assembly burnup in any X-Y cross-sectional plane is constant.
- The fuel exposure of the uppermost  $2$  ft and lowermost 2 ft of the fuel assembly is 80% of the fuel assembly average exposure.
- The fuel exposure of the middle  $8$  ft of the fuel assembly is 110% of the fuel assembly average exposure.

Output Specification. The output for this problem is the gamma radiation dose at the measurement points described earlier. The calculated gamma energy spectrum should be compared with that given in Table 4.2-7 for consistency. The gamma dose should be reported in units of R/hour or KR/hour for comparison with measured values.

Comments. This problem has not been simulated using a Monte Carlo Transport Theory code. Additional problem assumptions may be necessary to perform effective analyses. Reference JU-81 states that the measured results are reproducible to  $\pm 4\%$ . Fuel burnups are thought to be accurate to ± 3%. Dose rate instrumentation was biased 18% higher than a calibrated detection system. The reported standard error was ±12R/hour.

From Reference JU-81, we were not able to determine whether the units of the reported gamma dose are Roentgen/hour or Rad/hour (1 Roentgen =  $0.88$ ) Rad).

#### **4.3 Boiling Water** Reactor **Fuel** Assembly **Radiation Level**

Problem Statement. This problem presents the results of in-plant test measurements of the radiation field in air and water around a Boiling Water Reactor (BWR) fuel assembly. The problem is based on measurements taken at General Electric's Morris Operation.

Objective. This problem provides a basis for comparing the radiation field calculated using a source term code and a shielding code with measured experimental data.

Physical Description. Dresden Unit 2 uses General Electric 7x7 fuel assemblies. The fuel was irradiated from April 1970 (first significant power) to January 1971. After discharge from the reactor and cooling, the fuel was shipped to General Electric's Morris Operation for interim storage. As part of an engineering and test support contract funded by the Department of Energy, selected fuel assemblies were characterized. Gamma exposure rates near spent fuel assemblies were measured eight years after discharge of the fuel from the reactor.

Estimated fuel assembly operating conditions are given in Table 4.3-1. Fuel assembly design characteristics are presented in Table 4.3-2. The initial non-actinide composition of uranium fuel oxide pellets is given in Table 4.3-3. The weight of fuel assembly structural materials is presented in Table 4.3-4, and fuel assembly operating conditions are summarized in Table 4.3-5.

The concentrations of fuel assembly structural material located in the end fitting zone should be multiplied by 0.13 to account for the lower activation levels near the ends of the fuel assembly due to flux levels lower than those in the active fuel zone. In addition, the concentrations of manganese, cobalt, and zirconium in the end fitting zone should be multiplied by factors of 0.80, 0.67, and 0.32, respectively. These corrections account for the difference between the neutron energy spectrum in that zone and the spectrum in the active fuel zone. Both kinds of corrections are based on axial spectrum calculations for a General Electric BWR fuel assembly as reported in Reference CR-78. With these corrections, the ORIGEN-S calculations should more accurately predict the nuclide activities from the structural materials.

Reference JU-81 gives the results of experimental measurements of gamma dose rate and calculations using the shielding factor code QAD. These

# Table 4.3-1 -- In Development

 $\overline{\phantom{a}}$ 

Fuel Design Data for Dresden 2

Percent Theoretical Density<sup>a</sup> for UO<sub>2</sub> Initial Uranium Composition (wt.  $x$ )<sup>b</sup> 95.0 2.12



a Theoretical UO<sub>2</sub> density is 10.96 g cm<sup>-3</sup>.

- b Fuel assembly average 30 rods at 2.44%, 16 rods at 1.69%, and 3 rods at 1.20%.
- c Assuming a 35% void fraction.

 $\bar{z}$ 

 $\overline{\phantom{a}}$ 





a Parts of element per million parts of heavy metal.

b Stoichiometric quantity for M02 fuel, i.e., atom of U or Pu. two atoms of 0 per

C Average of 1,573 ppm of gadolinium in BWR fuel rods as a burnable poison.

Source: CR-78

 $\overline{a}$ 

#### Assumed Fuel Assembly Structural Material Mass Distribution in a BWR



Source: MI-83

# Fuel Assembly Operating Conditions



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results are given for measurements taken at several axial locations for the X-Y detector locations given in Table 4.3-6.

Table 4.3-7 gives the calculated intensities from Reference JU-81 for the gamma radiation source in spent fuel.

Table 4.3-8 gives the measured gamma exposure rates at the fuel assembly mid-point along the "Bl" profile for three fuel assemblies that were believed to have similar irradiation histories. In addition to measured exposures at each corner, Table 4.3.8 provides an indication of the anisotropy of gamma exposure. For irradiated fuel assemblies, the measured gamma exposure varied by as much as  $\pm 10\%$ . (In calculating the gamma intensity around a fuel assembly, it is commonly assumed that fuel burnup and therefore the gamma source is evenly distributed.)

Results of additional measurements made along the B1 profile at 1 ft intervals are given in Table 4.3-9. These measurements provide an estimate of the standard error of the expsoure rate measurement of about 9% (one sigma).

Table 4.3-10 gives results of calculated and measured exposure rates in air and water for three detector profiles.

Reference JU-81 includes a discussion of the accuracy and precision of measured results. Based on an analysis of all identified sources of random errors, the overall variability of measurements is estimated to be 9.1%. This reference also states that based on its measurements, a variance of  $\pm 3\%$  (one sigma) between utility-calculated fuel exposures and true exposures may exist. This agrees with generally held beliefs about the accuracy of these calculations and is consistent with IAEA guidelines established for safeguards purposes.

Assumptions. Analyses may be performed using the following assumptions:

The entire fuel assembly (except end fittings) is a homogeneous mass.

## Gamma Detector Locations



 $\overline{\ast}$  The origin is the corner of the fuel assembly envelope at the top of the active length of the fuel.

\*\* This detector is located above the fuel assembly.

Source: JU-81

#### Calculated Gamma Intensities for Gamma Radiation Sources in Spent Fue



Source: JU-81

# Exposure Rates from Fuel Assemblies

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Source: JU-81

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## Exposure Rate from Repeated Fuel Assembly Measurements



\*Distance from the top of the active fuel height.

Source: JU-81





\* Feet below top of fuel assembly active height.

Source: JU-81

The two center rows of fuel rods are modeled discretely, the remaining rods are homogenized.

Additional simplifying assumptions are:

- Spacer grids are homogenized over the entire assembly.
- Fuel assembly burnup in the X-Y plane is assumed to be equal.
- The fuel exposure of the uppermost 2 ft of the fuel assembly will be 50% of the fuel assembly average exposure.
- The fuel exposure of the lower 10 ft of the fuel assembly will be 110% of the fuel assembly average exposure.

Output Specification. The output for this problem is the gamma radiation dose at the measurement points described earlier. The calculated gamma energy spectrum should be compared with that given in Table 4.3-7 for consistency. The gamma dose should be reported in units of R/hour or KR/hour for comparison with measured values.

Comments. This problem has not been simulated using a Monte Carlo Transport Theory code. Additional problem assumptions may be necessary to perform effective analyses. Reference JU-81 states that measured results are reproducible to  $\pm 4\%$ . Fuel assembly burnups are thought to be accurate to ±3%. However, the axial burnup distribution of low exposure BWR fuel is not easy to estimate without performing coupled depletion/thermal-hydraulic analysis. Dose rate instrumentation was biased 18% higher than a calibrated detector system. The reported standard error was ±12R/hour.

From Reference JU-81, we were not able to determine whether the units of the reported gamma dose rates are Roentgens/hour or Rad/hour (1 Roentgen  $= .88$  Rad).

#### 4.4 Hypothetical Thin-Walled Waste Package Shielding Problem

Problem Statement. This problem requires the estimation of the gamma flux and neutron flux and dose around a hypothetical thin-walled, highlevel radioactive waste package. The hypothetical waste package is conceptually similar to packages that the Department of Energy has proposed for use in a salt repository. The flux and dose will be estimated at points within the shield and at points exterior to the shield.

Objective. The purpose of this problem is to provide a baseline for prediction of the gamma and neutron flux and dose in an environment similar to that which may exist around a waste package in a repository for high-level radioactive waste.

Physical Description. The waste package consists of a 2-3/4 in cylindrical carbon steel structural member covered by a 0.25 cm Ticode-12 overpack. Waste package design characteristics are summarized in Table 4.4-1. The gamma flux and dose rate are to be calculated at points in the structural component, in the Ticode-12 overpack, and at points in a salt host rock surrounding the waste package. Figure 4.4-1 shows a typical waste package emplacement environment.

Problem Solution. This problem will be solved using a transport theory computer program. It should be assumed that the spent BWR fuel rods had an initial enrichment of 2.7% and were irradiated at constant power over a three-year period to a discharge exposure of 27,000 megawatt days per metric ton of uranium. Subsequent calculations should be performed for time periods of 30, 100, 300, and 1,000 years following waste package emplacement.

Assumptions. In modeling the spent fuel rods contained in the waste package, it is adequate to analyze discretely the outermost two rows of fuel rods; The innermost fuel rods can be analyzed using the properties for a homogenized material composition. The problem may be analyzed in either one or two dimensions. Isotopic compositions of materials for this problem are given in Table 4.2-2.

## Table 4.4-1



## Summary of Waste Package Design Characteristics

 $\bar{z}$ 



Figure 4.4-1

Reference Spent Fuel Waste Package for Borehole Emplacement

Output Specifications. The outputs for this problem are the gamma photon flux and the neutron flux at the waste package centerline, at the outer carbon steel overpack surface, at the outer Ticode-12 surface, and at points 5, 10, 20, 50, 100, and 500 cm from the waste canister surface in the host rock.

Comments. This problem has not yet been analyzed. However, assessments performed by Westinghouse using a one-dimensional transport theory code estimated that the dose for 10-year cooled BWR fuel at the surface of the overpack would be approximately 106 millirems per hour.

#### **4.5 Hypothetical Thick-Walled Waste Package Shielding Problem**

Problem Statement. This problem requires the estimation of the gamma flux and neutron flux around a hypothetical thick-walled, high-level radioactive waste package. The hypothetical waste package is conceptually similiar to packages that the Department of Energy has proposed for use in the BWIP facility. The flux will be estimated at points within the shield and at points exterior to the shield.

Objective. This problem is designed to provide a baseline for prediction of the gamma and neutron flux in an environment similar to that which may be seen around a waste package in a repository for high-level radioactive waste.

Physical Description. The waste package consists of a 38 cm thick triangular cast iron container. Waste package design characteristics are summarized in Tables 4.5-1 and 4.5-2. The gamma flux is to be calculated at points in the waste package and at points in a bentonite backfill surrounding the waste package. Figures 4.5-1 and 4.5-2 show a typical waste package emplacement environment.

Problem Solution. This problem will be solved using a transport theory computer program. It should be assumed that the waste form is commercial

#### Table 4.5-1

### Summary of Alternate II (SSP) Waste Package Design Features



Cross Section Geometry Inside Dimension(s), cm Outside Dimension(s), cm Overpack Length, cm Overpack Empty Weight, tonne Overpack Loaded Weight, tonne Package Surface Radiation (mrem/hr) Modified Triangle 70 146 400 39.0 - 41.5 100

#### **Table 4.5-2**

### CHLW Characteristics



- (a) Glass refers to HLWin glass matrix.
- (b) These limits represent the glass softening point beyond which glass devitrification is possible.
- (c) This temperature limit may not be applicable to the NWRB where the backfill is used to control post-containment radionuclide release rates.
- (d) 24-day value. Leach rate is expected to go to 2 x 10-9 g/cm2 day after 400 days

Source: WE-82



# Figure 4.5-1

Reference Commercial High Level Waste Form





\*High **earben cotent et** eat kern **prowides** better neutron **attenuation: thas thimeer** wall Is **required.**

# Figure 4.5-2

# Typical Thick-Walled Waste Package

high-level waste from PWR fuel with an initial enrichment of 3.5% irradiated at constant power over a three-year period to a discharge exposure of 35,000 MWD/MTU. Calculations should be performed for waste cooling times of 10, 30, and 100 years following spent fuel discharge.

Assumptions. The problem may be analyzed in either one or two dimensions. Isotopic compositions of materials in this problem are given in Table 4.5-3.

Output Specifications. The outputs for this problem are the gamma photon flux, gamma photon dose, the neutron flux, and the neutron dose at the points given in Table 4.5-3.

Comments. This problem has not yet been analyzed. However, assessments performed by Westinghouse using a one-dimensional transport theory code estimated that the dose for 10-year cooled commercial high-level waste at the surface of the overpack would be approximately 100 millirems per hour.

## Table 4.5-3 -- In Development

#### 5.0 EMPIRICAL CORROSION AND LEACHING PROBLEMS

This section contains two verification problems for corrosion and leaching that can be used in the verification of the computer code WAPPA. Although the problems in this section are useful in showing that certain parts of the numerical algorithms of the code WAPPA function as designed, the code WAPPA relies heavily on empirical data, and its predictions will never be better than the empirical constants used in the code.

The first problem is based on test problems developed under the SCEPTER project. This problem is designed to allow sensitivity analyses on selected input parameters related to corrosion and leaching. The second problem is an analytical solution for solute transport by diffusion across an infinitely long cylindrical segment. This problem can be used to assess the acceptability of WAPPA's backfill leaching calculation.

#### **5.1 Simple** and **Complex Waste Package** Concepts **Used in the Verification of the WAPPA Code**

Problem Statement. The 7 barrier and 17 barrier test problems used in the verification of the WAPPA code under the SCEPTER project will be used to benchmark WAPPA. The simple and complex test problem configurations are summarized in Tables 5.1-1 and 5.1-2 respectively. Once the test problem results have been found to agree with those obtained under the SCEPTER project, the code will be run a number of times with selected changes made to the inputs related to corrosion and leaching. These changes will be within the range of uncertainty commonly associated with these data values.

Objectives. The first objective of this problem is to ensure that the version of the code on hand can reproduce the results from the earlier verification study. A more important objective, however, is to evaluate the sensitivity of code results to changes in corrosion and leaching parameters and uncover possible errors in the program logic which could be revealed by these changes.

# Table 5.1-1

# Verification Test for a Simple Waste Package Concept



 $\ddot{\phantom{a}}$ 

# **Table 5.1-2**





 $\ddot{\phantom{a}}$ 

Analytical Solution. The solution to this problem can not be expressed analytically.

Assumptions. The assumptions are identical to those of the WAPPA code (see Reference MI-83 for a description).

Input Specifications. The input data for the simple and complex configurations are listed in Appendix A.

Output Specifications. In addition to an echo print of input data and data base values, the output will include:

- . Barrier radii
- Temperature as a function of radius
- Ratio of the heat energy generated or deposited in a barrier or in the waste package to the total heat energy generated in the waste package
- Barrier status (intact, breached, or failed)
- Areal degradation factor
- Nuclide concentrations

#### **5.2 Solute Transport by Diffusion Across an Infinitely Long Cylindrical** Segment

Problem Statement. A constant flux of F and a constant concentration of zero are specified for the inner and outer surface, respectively, of an infinitely long cylindrical segment (see Figure 5.2-1) with inner radius a and outer radius b. The solute diffusion coefficient, D, is assumed to be constant throughout the segment. No solute is assumed to be present in the segment initially. The values to be calculated as a function of time are (1) the concentration profile across the segment, (2) the average concentration within the segment, and (3) the concentration gradient at the radius b.



$$
C(r, o) = 0 \qquad r >
$$

# Figure 5.2-1



Objectives. This problem is designed to test the backfill leaching calculation used in WAPPA and the assumption that the backfill can be treated as a single, uniformly mixed cell.

Analytical Solution. The concentration of solute as a function of time can be described by the diffusion equation in cylindrical coordinates:

$$
\frac{3^2C}{ar^2} + \frac{1}{r} \frac{aC}{ar} = \frac{1}{D} \frac{aC}{at}
$$

(148)

with the following boundary conditions:

$$
-D\left(\frac{\partial C}{\partial r}\right)_{r=a} = F(a constant)
$$

$$
C(b,t) = 0
$$
  
C(r,0) = 0 for r  $\ge a$ 

The analytical solution to this equation is given as follows:

$$
C(r,t) = \frac{aF}{D} \ln \left(\frac{b}{r}\right) + \frac{\pi F}{D} \sum_{m=1}^{\infty} exp(-D\alpha_n^2 t) x
$$

$$
\frac{J_0^2(b\alpha_n) \left[J_0(r\alpha_n)Y_1(a\alpha_n) - Y_0(r\alpha_n)J_1(a\alpha_n)\right]}{\alpha_n \left[J_1^2(a\alpha_n) - J_0^2(b\alpha_n)\right]}
$$

(149)

where  $\alpha_n$  are the positive roots of

-

$$
J_1(a\alpha)Y_0(b\alpha) - Y_1(a\alpha)J_0(b\alpha) = 0
$$

Assumptions. There is no variation of solute concentration with the angle or along the axis of the cylindrical segment. Also, solute advection, adsorption, and decay within the segment are neglected.

Input Specification. Calculations are to be performed for a wide range of values of inner radius a, outer radius b, diffusion coefficient D, and flux F at radius a.

Output Specifications. The solute concentration as a function of time is calculated for a range of distances between a and.b. Also, the average concentration within the cylindrical segment is calculated as a function of time. Finally, the concentration gradient at  $r = b$  is calculated as a function of time. Concentration profiles for different values of b/a were calculated by use of Equation 149 and are displayed in Figures 5.2-2 through 5.2-4. The associated average concentrations and concentration derivatives at  $r = b$  are given in Table 5.2-1. In reporting these results, all concentrations, distances, and times have been normalized as indicated in Figures 5.2-2 through 5.2-4.


Figure 5.2-2





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201



**Figure 5.2-4**

Normalized Concentration Curve for  $B/A = 8$ 

202

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### **Table 5.2-1**

#### Average Normalized Concentrations and Boundary Derivatives for Different Values of b/a\*



\* Results based on the evaluation of 40 terms in the Equation 149 summation.

\*\* Slope based on the last two points plotted in each of the Figures 5.2-2 through 5.2-4.

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#### 6.0 WASTE PACKAGE GEOCHEMICAL CODE BENCHMARK PROBLEMS

Numerical models may be used to simulate geochemical processes in the high-temperature regions around waste packages in a nuclear repository. Benchmarking the geochemical codes that may be considered for such use requires appropriate test problem data sets. Ideally, a test problem will evaluate the utility of each code and verify the code algorithms for the geochemical processes being modeled.

Geochemical models should provide input to analyses of the effects of near-field geochemistry on waste form solubility and leaching, canister corrosion, and backfill properties. The usefulness of geochemical models to the analysis of these effects will depend not only on the development of the necessary algorithms and thermodynamic data, but also on the data to verify and validate the codes.

Since there is no direct experience with the complex interactions of high-level waste packages with backfill material, host rock, and groundwaters, data must be obtained from other sources. For example, laboratory studies have been conducted on representative samples of waste form, canister backfill, and host rocks related to repository media (References AP-82, CH-83a and b, GO-81, GR-83, KE-84, KU-81, MO-83, MY-83, RE-82, SE-84, and WO-82). Laboratory studies may provide useful information as controlled experiments, although certain drawbacks exist. For example, problems in laboratory methods raise significant questions about the usefulness and viability of some early experiments (References KE-84 and CR-84).

Shortcomings in laboratory experiments often arise from difficulty in formulating synthetic groundwater representative of that found in the candidate host rock; obtaining unaltered, representative samples of repository rock; and reproducing the temperature, redox, and degree of openness of the system. In addition, laboratory-scale tests are restricted in time, raising the possibility that kinetically controlled reactions will prevent the attainment of equilibrium conditions, an all-important

assumption with state-of-the-art geochemical models. For these reasons, laboratory experiments have not been utilized as potential test problems in benchmarking equilibrium-based geochemical models.

If the methodological problems can be surmounted, laboratory experiments may prove to be valuable test problems for the benchmarking of kinetically based geochemical models now in the developmental stage. A kinetic benchmark problem is offered in Problem 6.5 in anticipation that a kinetic model may be developed. Even here, an understanding of the long-term behavior of repository systems over hundreds of years may be satisfied only partially by such short-term experiments (Reference EL-83).

One approach to dealing with uncertainties in extrapolating from the laboratory scale to the repository scale (both in time and space) is to investigate comparable geologic systems found in nature. These "natural analogs" may contribute to understanding the processes that will occur in a repository over many hundreds of years (Reference EL-83):

- The Oklo, Gabon, uranium ore body achieved criticality naturally about two billion years ago. Researchers have measured the extent of migration of radionuclides similar to those derived from high-level waste.
- Metamorphic haloes surrounding igneous intrusives can be studied to observe the effects of heat on clay backfill and host rock.
- Metamict effects on minerals show crystal structure damage from radiation.
- . Geothermal systems allow the study of mineral alteration products due to elevated temperatures.

Natural analogs that are similar to geochemical processes in high-level radioactive waste repositories should provide fairly complete data on the chemistry of water, mineralogy, and effects of changing temperature. Temperature and pressure of the natural analog should be in the range of 500 -3000C and up to about one hundred bars of hydrostatic pressure. Ideally, stable mineral assemblages under known water chemistry and

temperature conditions should be well documented. The natural analog selected for a given candidate repository also should exhibit petrology, mineralogy, and groundwater chemistry similar to those of the candidate repository.

Based on these criteria, proposed natural analogs may be selected for use in the development of geochemical code benchmark problems. A search of the literature has revealed that sufficiently detailed studies of the geochemistry of geothermal systems are available to provide potentially valuable natural analogs. With temperature typically ranging from ambient to over 3000C and pressures under hydrostatic conditions ranging up to about one hundred bars, geothermal systems provide natural analogs of water-rock interactions within a pressure and temperature range similar to that anticipated for high-level waste repositories. In addition, the variety of geologic terrains in which geothermal systems occur provides petrologic, mineralogic, and hydrogeochemical conditions similar to those in the candidate repository media under consideration. Table 6-1 lists several geothermal systems, the host rock to which they are similar, and a qualitative rating of the degree to which they have been studied.

The candidate media for a deep geologic repository for high-level waste in the United States include at least four rock types\*:

- 1. Basalt (Hanford Reservation, Washington)
- 2. Tuff (Nevada Test Site)
- 3. Salt (Gulf Coast salt domes and bedded salt in Palo Duro Basin, Texas, and Paradox Basin, Utah)
- 4. Granite (not selected yet)

In addition, the United States is involved in research on the feasibility of seabed disposal. This research is conducted jointly with seven other countries under the auspices of the Nuclear Energy Agency of the Organization for Economic Cooperation and Development.

### **Table 6-1**





\*Level of study refers to a subjective evaluation of the amount of research and the degree of understanding of the system.

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Although the DOE has devoted most of its efforts to studying the basalt site at the Hanford Reservation (BWIP), the tuff site at the Nevada test site (NTS), and bedded and dome salt sites, the Department has initiated the screening process to select candidate sites in granite for further study. Furthermore, the DOE is well along in the evaluation of bedded salt at the Waste Isolation Pilot Program (WIPP) in New Mexico.

These potential media present different problems in understanding the physical and chemical processes that will control the repository environment. Rock types being considered include mafic (basalt) and silicic (rhyolite and granite) igneous rocks, sedimentary evaporites (bedded salt), and diapiric salt domes (Gulf Coast salt domes).

In the near-field environment of a repository, consisting of a waste package and backfill emplaced within a mined opening, geochemical interactions must be simulated in an environment where temperature may rise as high as 2000-3000C for several years, then gradually decline over several hundred years as shown in Figure 6-1 for the spent fuel case in a basalt repository (Reference RO-82).

During the life of a basalt repository, the near-field environment will initially be under oxygenated, dry conditions. As the temperature drops, resaturation is predicted to occur after 360 to 390 years (Reference RO-82), and anoxic conditions will return.

Thus, during the early, unsaturated high-temperature period, dehydration will be the most important process, while after resaturation of the backfill and host rock, water-rock interactions will be important, especially at elevated temperatures.

To simulate geochemical processes in a changing thermal regime requires not only that the aqueous speciation, redox potential, and degree of mineral saturation be calculated but also that temperature effects be



Figure 6-1

Temperature-Versus-Time Curves for Different Components of a Vertically Emplaced Spent-Fuel Waste Package in a Repository Located in Basalt (RO-82)

incorporated. Therefore, the benchmark problems have been designed to test the effects of temperature within the full range expected for the near-field, as well as to test the algorithms for deriving speciation, redox, and saturation indices. In addition, some geochemical codes (reaction path models) may be used to simulate water-rock interactions in systems that have changed from one equilibrium condition to another, either through heating or cooling or through the migration of water to a different mineral regime.

The benchmark problems designed for near-field geochemical codes are:

4,



- Problem 6.3: Hypothetical radionuclide equilibrium speciation and mineral solubility
- Problem 6.4: Reaction path incorporating effects of changing temperatures on mineral-water equilibria
- Problem 6.5: Reaction kinetics based on experimental results

#### **6.1** Low-Temperature (<1500C) Basalt Analog **without Boiling**

Problem Statement. This problem requires the calculation of aqueous speciation, mineral saturation indices (SI), and redox potential (Eh) for a low-temperature (<1500C) geothermal groundwater. The temperaturepressure conditions are such that only two phases, liquid and solid, are considered. Coexisting mineral assemblages for the groundwater are presented as confirmation of the calculated SIs.

Objective. This problem provides a benchmark test of the routines for solving the equilibrium aqueous speciation and mineral solubility products or saturation indices for a two-phase, liquid water-rock system at a temperature of 1000-1500C.

Physical Description. This problem uses the data presented by Arnorsson and his coworkers (References AR-78, AR-82, and AR-83) on the hydrogeochemistry of the geothermal fields in southwest Iceland. Both the fluid chemistry and hydrothermal mineral alteration of this region have been studied intensely.

Table 6.1-1 presents a comparison of the range and average major-element composition of the middle Sentinel Bluffs and Umtanum flows and Icelandic basalt. This comparison indicates that, although there are variations in the percent distribution of the oxides of major elements, especially magnesium, the basaltic rocks of the Grande Ronde and Iceland are essentially similar, especially considering that the ranges overlap for most oxides. In comparing altered versus unaltered Icelandic basalts, Kristmannsdottir (Reference KR-75) found that the major changes in the altered rock are hydration and oxidation, with enrichment of SiO<sub>2</sub> in some samples.

The comparison of groundwater chemistry between the Grande Ronde and Icelandic basalts is presented in Table 6.1-2. The groundwater chemistry is very similar, although minor variations are again present. The Icelandic waters tend to be slightly more dilute with a mean total dissolved solids (TDS) content of almost 400 milligrams per liter (mg/l) while the Grande Ronde averages 900 mg/l. The maximum TDS in both the Icelandic and Grande Ronde samples is about 1,000 mg/l.

A major difference between the two waters is the fluoride content. The Icelandic groundwaters have only about 2 mg/l of fluoride, on average, while the Grande Ronde groundwaters have 8 to 16 times as much. This probably is due to a greater abundance of apatite minerals, although there is some question about apatite as the source of fluoride in Grande

### **Table 6.1-1**

#### Comparison of Major-Element Composition of Basaltic Rock of the Umtanum and Middle Sentinel Bluffs Flow at the Hanford Site with Basaltic Rock of Southwest Iceland (in weight percent)



a From Reference RO-82, Table 6.1.

b Calculated from data in Reference KR-75, Tables 1 and 2.



#### Major Ion Chemistry of Groundwaters Hanford Site Compared to the in the Umtanum and Middle Sentinel Bluffs Flow at Geothermal Waters in the Icelandic Basalts

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Ronde groundwater (Reference RO-82). Finally, the pH and temperature range of the Icelandic groundwater represented in Table 6.1-2 bracket the ranges for the Grande Ronde analyses.

Alteration zones, or stable mineral assemblages versus temperature, have been described for the Icelandic geothermal systems (References KR-75 and AR-83). In general, for the low-temperature systems ( $<150^{\circ}$ C), four zones of mineral alteration have been established based on temperature. Figure 6.1-1 presents the alteration zones described by Kristmannsdottir (Reference KR-75).

Although the temperature ranges of the zones in Figure 6.1-1 are very approximate, they do provide an estimate of the stable mineral assemblages that would be anticipated in the Icelandic basalts under low-temperature conditions. Even though this figure shows zones for only two locations in Iceland, comparison to other areas in Iceland has shown similar alteration zones (Reference KR-75).

Chabazite (a zeolite) and opal with minor calcite, levyne (a zeolite), smectite, and mixed-layer clays characterize Zone I in the temperature range up to about 700-800C. Between 700-800C and about 900C, mesolite and scolecite (zeolites) are the alteration minerals characteristic of Zone II. Calcite and smectite also are found in Zone II along with minor amounts of several other zeolites and mixed-layer clays. Zone III occurs between about 900C and 1100-1200C and is characterized by the dominance of the zeolite stilbite. Above about 1200C, Zone IV is characterized by laumontite, the stable zeolite, along with quartz, calcite, smectite, and minor mixed-layer clays.

#### Assumptions.

- The water sample represents a water from a single horizon.
- The water sample did not boil.



## Figure 6.1-1

Alteration Mineral Zones found in the Reykjavik and Reykir Low-Temperature Area. The Rock Temperatures of the Zone Borders are Very Approximate (KR-1975)

- The mineral assemblage represents prograde alteration only.
- The water and minerals are at equilibrium.
- The redox system is at equilibrium and well poised.
- The Debye-Huckel theory adequately describes non-ideal behavior of dissolved ions.
- Mineral dissolution is congruent.
- Minerals are stoichiometric.
- The water has not interacted with casing or minerals nor solutes precipitated out of solution on the way to the surface.
- No degassing of the water sample occurred.

Input Specifications. The input data consist of measurements made on the surface. The input data for the low-temperature benchmark problem are presented in Table 6.1-3.

Output Specifications. The output for this problem will include the activity coefficients of the solutes, molal activities of aqueous species, ionic strength, ionic balance, Eh based on the H2S-S04 redox couple, temperature based on the quartz and sodium-potassium geothermometers, and solubility products or saturation indices of important minerals.

**6.2** Three-Phase, High-Temperature (>1500C) **Equilibrium Speciation**

Problem Statement. This problem requires the calculation of aqueous speciation, mineral saturation indices (SI), and redox potential (Eh) for a high-temperature (>1500C) geothermal groundwater. The temperaturepressure conditions are such that the water boils as it is withdrawn from the well prior to sampling. The model must calculate the geochemistry (i.e., temperature, aqueous speciation, SI, and Eh) of the water as it occurs in the aquifer. Alteration mineral assemblages for the host rock are presented as a confirmation of calculated SIs.

### Table 6.1-3

Input Data for Low-Temperature Basalt Analog Benchmark Problem (Reykjavik, Iceland, Well 11)



Source: Reference AR-82

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Objectives. This problem is a test of the routines for calculating the activity coefficients, aqueous speciation, ionic strength, ionic balance, Eh based on the H2S-S04, CH4-C03, H2-H20, and NH3-N03 redox pairs; and the solubility products or saturation indices for important minerals in a three-phase, steam-water-mineral system. The problem'also requires the code to back-calculate the original, in-situ chemical composition of the water by incorporating the chemical data on the steam sample collected with the water sample.

Physical Description. This problem uses the data presented by Arnorsson, et al., (Reference AR-82) on the analyses of the Krafla geothermal field (Well 7) in northern Iceland. Well 7 is 2,165 m deep, with producing zones at 825, 1,163, 1,700, and 2,000 m, having temperatures of 160, 206, 287, and 3400C, respectively. The chemical analysis for Well 7 is presented in Table 6.2-1.

The stable mineral assemblage for high-temperature geothermal systems determined from core samples in Iceland is presented in Figure 6.2-1. Minerals that may occur at temperatures over 2500C include quartz, calcite, fluorite (which may not be present), anhydrite, low albite, microcline (potassium feldspar), mixed-layer clays, chlorite, wairakite or prehnite, pyrite, iron hydroxides, and epidote.

#### Asssumptions.

- . The water sample represents water from a single horizon.
- Flashing to steam due to pumping does not extend into the aquifer.
- The mineral assemblage represents prograde alteration only.
- The water and minerals are at equilibrium.
- . The redox system is at equilibrium and well poised.
- The water has not interacted with or precipitated any substances on its path to the surface.
- The amount of degassing of the water sample can be closely estimated.



Input Data for High-Temperature Basalt Analog Benchmark Problem (Krafla, Iceland, Well 7)



Source: Reference AR-83



1 Modified from AR-83 and KR-75.

2Upon cooling when under 1000C, analcime may become stable, especially in olivine basalts.

3Smectite gradually alters to chlorite between 200-2400C via mixed layer clay minerals. Mixed layer clays begin to appear at about 1000C.

4May also have prehnite.

## **Figure 6.2-1**

Empirically Determined Stable Mineral Assemblages for Geothermal Waters in Icelandic Basalts in the Temperature Range of 0-300°C and Pressure Less Than 14 MPa

Input Specifications. The input chemical data for this problem are presented in Table 6.2-1.

Output Specifications. A solution to this problem has been calculated previously (Reference AR-82) and is presented in Table 6.2-2, which lists the input data (i.e., the chemical analysis and deep-water temperature and pressure); the calculated deep-water chemistry after the vapor phase is recombined with the liquid; and the activity coefficients for the various species, the activities, ionic strength, ion balance, geothermometric temperatures, Eh, and the solubility products for 26 minerals. Table 6.2-3 lists the saturation indices (SI) computed from data in Table 6.2-2 and compares the SI values with the mineral assemblage determined empirically.

#### **6.3 Hypothetical Radionuclide Equilibrium Speciation and Mineral Solubility**

Problem Statement. This test problem presents data on a hypothetical case involving the determination of solubility contols under high temperatures on radionuclides in groundwater in clastic sedimentary strata. This problem requires the calculation of aqueous speciation and mineral saturation indices for major constituents and radionuclides at temperatures ranging from ambient (500 to 1000C) to a maximum of about 4000C. Pressures vary from about 30 to 300 MPa.

Objectives. This test problem serves as a benchmark of a geochemical code for the calculation of the aqueous speciation and mineral saturation indices for radionuclides in a high-temperature environment similar to the near-field.

Problem Description. The Oklo uranium ore district in Gabon, Africa, reached criticality through natural processes about two billion years ago and maintained a nuclear reaction for an estimated 500,000 years. The ore formed initially at about the same time as the formation of the host

### Table 6.2-2

#### Output of the Program WATCHI Showing Original Input Data, Correction of Surface Sample to Deep Water, and Calculation of Aqueous Speciation and Solubility Products for 26 Minerals



(continued)

## Table 6.2-2 (continued)



Gas Solubility Multiplying Factor: 0.10

(continued)

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0.834

ACTIVITY COEFFICIENTS IN DEEP WATE





(continued)

Table 6.2-2 (continued)



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 $\label{eq:2} \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^{2} \left(\frac{1}{\sqrt{2}}\right)^{2} \left(\frac{$ 

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 $ATHEOR = Logarithm of the theoretical solubility product at equilibrium, which is equivalent to the$ logarithm of the equilibrium constant (log K).

bCALC = Logarithm of the calculated solubility product (log Q).

Source: Reference AR-82



### **Table 6.2-3**

Calculated Mineral Saturation Indices (SI) for Benchmark Problem 6.2 and Comparison with Empirical Stable Mineral Assemblages from Figure 6.2-1

## $a SI = log Q - log K$

b **'"+"** means mineral is generally present, and a blank means it is absent at the temperature range under consideration.

rock, an argillaceous sandstone-shale-carbonate-conglomerate sequence named the Francevillian Series. The primary host rocks were argillaceous sandstones and sandy shales. Tilting and fracturing of the host rock soon after its formation created open fractures that were later filled in with clay. At about the same time, the uranium ore in the argillaceous sandstone was remobilized. As the remobilized uranium migrated through the clay-filled fractures, reducing conditions caused the uranium to precipitate, resulting in an enriched pitchblende of 50 to 70 percent uranium content. Major gangue minerals associated with the enriched ore include chlorite, illite, carbonates, barite, chalcopyrite, pyrite, and hematite (Reference BR-84a).

During the nuclear reactions that occurred, temperatures in the ore body are thought to have reached over 4000C while, in the host rock, the temperatures probably remained under 2500C and rapidly decreased away from the ore body. It has been estimated that temperatures beyond 1 m of the ore body were below 2000C (Reference BR-84a). The ambient temperature of this region is thought to range from 50° to 1500C due to a regional geothermal gradient of 400-500C per kilometer of depth (Reference BR-84a).

Although no data on groundwater chemistry are known to have been published, or collected (Reference BR-84b), some idea of the ambient groundwater quality has been formulated. The Oklo hydrothermal system was low in chloride, ammonia, and cyanide and relatively low in sulfur (Reference BR-84b).

Since there are similarities between the primary Oklo ore genesis and the uranium ore genesis in the Grants Mineral Belt of New Mexico, it is possible to construct a hypothetical groundwater analysis for the Oklo site prior to the nuclear reaction. Table 6.3-1 presents a typical chemical analysis for groundwater from the Westwater Canyon Member of the Morrison Formation in the Grants Mineral Belt. The depth of samples comparable to that in Table 6.3-1 is about 250 m. This analysis compares favorably with the qualitative estimates of Brookins (Reference BR-84a) as stated above.



Chemical Analysis of Groundwater from the Westwater Canyon Member of the Morrison Formation, Grants Mineral Belt, New Mexico

Table 6.3-1

Source: Modified from Reference ST-83

Brookins (Reference BR-84a) has developed Eh-pH diagrams for several constituents. Figure 6.3-1 presents an Eh-pH diagram for the system uranium-silicon-sulfur-carbon-hydrogen-oxygen at 250C and 1 bar (105 Pa) pressure. The stability region for uraninite  $(100<sub>2</sub>)$ , the ore in both the Oklo and Grants districts, is in the pH range of about 7 to 9 and the Eh range below about -0.1 volts.

#### Assumptions.

- The hypothetical chemical analysis presented in Table 6.3-1 represents an analysis of major chemical components in groundwater of the Francevillian sedimentary rocks at Oklo.
- The pH-Eh can be approximated from the stability diagram of Figure 6.3-1.
- Equilibrium between minerals and solution is maintained at all temperatures in the hypothetical system.
- The production and release of fission products at Oklo can be approximated as an instantaneous event (this is a reasonable assumption considering the 2 billion year total time scale).
- The temperature of the pitchblende immediately  $\bullet$ increased to 4000C. A zone out to about 1 m attained an average temperature of 2500C, and beyond about 1 m from the ore, the temperature was ambient.

Input. The initial input data for the test problem are presented in Table 6.3-1. The beginning mineral assemblage is quartz, chlorite, illite, carbonate, barite, chalcopyrite, pyrite, hematite, and pitchblende.

Fission products include those listed in Table 6.3-2.

Output. The output consists of activities of aqueous species for the major constituents listed in Table 6.3-1 and the products listed in Table 6.3-2. Mineral saturation indices for solid phases incorporating those constituents are calculated.





Eh-pH Diagram for Part of the System U-Si-S-COH-O at  $25^{\circ}$ C and  $10^5$  Pa Pressure (BR-84)

### Table 6.3-2

### Fission and Nonfission Products from the Oklo Nuclear Reaction

Selenium Bromine Rubidium Strontium Yttrium Zirconium Niobium Molybdenum Technetium Ruthenium Rhodium Palladium Silver Cadmium Indium Tin Antimony Tellurium Iodine Xenon Cesium Barium REEab Lead Bismuth Thorium Uranium Transuranicsb

a Rare earth elements

b Transuranic elements and REE are each combined since the elements in each group behave similarly.

For comparison, studies of the Oklo site have indicated the relative mobility of the reaction products. Based on field observations and predictions from Eh-pH diagrams, Brookins prepared the analyses presented in Table 6.3-3 (Reference BR-84a).

#### 6.4 Reaction-Path Problem with Cooling

Problem Statement. This problem requires the calculation of aqueous speciation, mineral saturation indices, and the mass transfer of minerals and gases as the result of cooling along the flow path for a hightemperature brine. Comparisons between predicted and observed water chemistry and between predicted mineral-water reactions and known mineralogy serve to validate the geochemical mass transfer code.

Objectives. The features of the code being tested are the calculations of aqueous speciation, activities of species, mineral saturation, mass balance, and mass transfer. The mass transfer calculations predict the reactions of minerals and gases within the water-rock system and the associated transfer of mass into or out of the aqueous solution. Predictions of mineral dissolution, precipitation, or alteration are considered a function of temperature.

Problem Description. A geochemical model of the evolution of deep-sea brines in the Red Sea geothermal systems by Shanks and Bischoff (Reference SH-77) is used as a near-field test problem for the benchmarking of reaction-path geochemical models. The problem involves the analysis of the geochemistry of a natural geothermal brine and the subsequent alteration of that brine as it cools, but does not mix with Red Sea waters, upon exiting the subsurface at the bottom of the Atlantis II Deep in the central Red Sea. The changes in the brine chemistry are to be used in the predictions of mass transfer, i.e., mineral precipitation or dissolution, that occurs during cooling.

Although accurate determinations of the subsurface brine are not available, data for deep Red Sea brine just above the sediment-water interface have allowed the extrapolation back to the original brine chemistry

### Table 6.3-3



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### Observed Mobility of Important Elements at Oklo Compared to Predicted Mobilities Based on Eh-pH Diagrams

(continued)

# Table 6.3-3 (continued)

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Source: Reference BR-84a

 $\sim$ 

 $\sim 10^{-1}$ 

 $\sim$ 

 $\sim 10^7$ 

 $\mathcal{A}$
and temperature. The brine chemistry in the lower layer of the Red Sea in Atlantis Deep II has a chlorinity of 156 parts per thousand and essentially represents original brine unmixed with sea water (Reference SH-77).

The initial brine temperature has been estimated by several methods to range from 150-2610C. A temperature of 2500C for the original geothermal brine has been assumed (Reference SH-77). The temperature of the brine after entering the Red Sea has been measured at 60°C.

A second major assumption concerns the presence of hydrogen. Although hydrogen sulfide has not been detected in the brine, some sulfide minerals are forming. Since the sulfate concentration (840 ppm) in the brine is high, the hydrogen sulfide concentration should be very low (Reference SH-77).

The sulfate-sulfide equilibrium distribution and the concentration of sulfide species can be obtained from the oxygen fugacity determined by the magnetite-hematite equilibrium:

 $3Fe<sub>2</sub>O<sub>3</sub> = 2Fe<sub>3</sub>O<sub>4</sub> + 1/2 O<sub>2</sub>$ Hematite Magnetite

#### (150)

The temperature-dependent equilibrium constant for this reaction can be determined from the data supplied by Helgeson (Reference HE-69).

Finally, the pH of the brine as a function of temperature has been estimated using an experimentally determined pH of 5.5 for cooled brine samples at 250C, plus a mass balance relation for hydrogen-bearing species at higher temperatures.

The reaction path model requires the calculation of saturation indices to indicate the controlling mineral-water reactions. Mass balances for those controlling reactions are calculated to determine the mass transfer

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such that the change in the number of moles of an aqueous species along a flow path is equal, but of opposite sign, to the change in moles of the solid mineral phases that incorporate that species. In this case, the flow path is from the subsurface region with a temperature of 2500C to the Red Sea brine at the sediment-seawater interface where the temperature of the brine has cooled to 600C.

Assumptions. All the assumptions of the reaction path model incorporate those of the equilibrium speciation model:

- Homogeneous equilibrium is maintained throughout the reaction paths.
- . The Debye-Huckel theory adequately describes the non-ideal behavior of dissolved ions.
- Mass and charge are conserved.
- Mineral dissolution is congruent.
- Mineral formulas are stoichiometric.

In addition, it is assumed for this test problem:

- That the maximum temperature of the original brine  $\bullet$ is accurately estimated to be 2500C
- That the activity of hydrogen sulfide can be accurately estimated from the oxygen fugacity that is fixed by the magnetite-hematite equilibrium
- That the oxygen fugacity determined as a function of temperature is valid
- . That the pH as a function of temperature can be accurately estimated on the basis of the empirical method described above
- . That the overall chemical composition of the brine has not changed

Input. The input data are presented in Table 6.4-1.

## Table 6.4-1

## Input Data for the Red Sea Brine



Source: Reference SH-77

Output. Output for this test problem includes aqueous speciation and activities, mineral saturation indices (ion activity product divided by the equilibrium constant), and mass transfer calculations. The mass transfer calculations will consist of changes in the mass of each dissolved constituent per unit mass of water (i.e., moles per kilogram of water).

As a partial validation, saturation indices for important minerals have been calculated as a function of temperature (Reference SH-77) and are presented in Figure 6.4-1.

#### 6.5 Reaction Kinetics Problem

Problem Statement. This problem requires the solution of the rate of change over time in the concentration of an aqueous species or the rate of change over time in the mass per unit volume of a solid. The rate of change in concentration or mass is to be solved at an elevated temperature. Experimental results are provided for comparison.

Objectives. The features of a kinetics code being tested are the data base of rate constants utilized for the reactions, the temperature functions of the rate constants, and the aqueous speciation and activities under nonequilibrium conditions.

Problem Description. Experimental work has been completed on the waterrock-spent fuel interactions under controlled temperatures ranging from IOOOC to 3000C and 30 MPa (Reference MY-83). The experimental method involved an essentially closed system using gold bags heated in an autoclave. During the run of an experiment, samples of fluid were periodically withdrawn for chemical analysis. The ratio of groundwater to basalt to simulated spent fuel was 20:1:1.

Alteration minerals observed in the experimental mixture of groundwater, basalt, and simulated spent fuel included saponite (smectite), illite, microcline, and poorly crystalline silica. The spent fuel was largely unaltered except for a surface alteration product that was tentatively

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Figure  $6.4-1$ 

Degree of Saturation of the Red Sea Geothermal Brine with Respect to<br>Various Hydrothermal Minerals, Expressed as a Ratio of Ion<br>Activity Product to Solubility Product Constant (IAP/Ksp)<br>For Each Mineral (SH-77)

identified as weeksite  $(K_2(U_2)_2(S_1)_3.4H_2O)$  or boltwoodite  $(K_2(00_2)_2(Si0_3)_2(0H)_2.5H_2O)$ . A minor amount of scheelite (CaWO4) also was detected as an alteration product.

Results of the chemical analyses indicated concentrations arrived at approximate equilibrium values in the closed system during the run of the experiments (Reference MY-83).

#### Assumptions.

- The experimental method represents a closed system. Fluid samples withdrawn periodically are small enough so that the overall chemical composition of the fluid is not affected.
- The closed system of the experimental setup approximates the real physico-chemical conditions of the near-field environment, i.e., fluid residence times are very long and local equilibrium between solution and minerals is approached.
- Experimental apparatus is inert with respect to all components in the simulated spent fuelgroundwater-basalt mixture.
- Simulated components such as spent fuel and groundwater are representative of the actual components.

Input. The mass ratio of the spent fuel to groundwater to basalt is 1:20:1. Three constant temperature conditions, 1000, 2000, and 3000C, and a single pressure condition, 30 MPa, are applied to the experimental mixture.

The basalt is from the entablature of the Umatanum flow of the Grande Ronde Basalt with the chemical and mineralogic composition shown in Table 6.5-1.

The synthetic groundwater, representative of that occurring in the Grande Ronde Basalt, has the chemical composition presented in Table 6.5-2.

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## Table 6.5-1

Chemical Analysis of Grande Ronde Basalt Sample RUE-1

Source: Reference MY-83

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Composition of Synthetic Groundwater

Source: Reference MY-83

The simulated spent fuel chemical composition is presented in Table 6.5-3.

Output. The output consists of the change in concentration over time of aqueous species, the dissolution/precipitation rates of initial solidphase components, and the precipitation rates of new solid-phase components.

Figure 6.5-1 presents results of experiments on the pH as measured in a sample cooled to 250C, and Figure 6.5-2 presents the pH values as corrected to the original temperature of 1000, 2000, or 3000C (Reference MY-83).

Figure 6.5-3 presents plots of concentration in solution versus time for sodium and silicon at the three temperatures. Figures 6.5-4 through 6.5-7 present similar plots for chloride and sulfate, iodine, strontium and uranium, and cesium and molybdenum, respectively.

## Table 6.5-3



## Chemical Analysis of Simulated Spent Fuel\*

\* Minor components have been tabulated as the element for use in inventory calculations.

Source: Reference MY-83











Effect of Temperature on Calculated pH Values for Simulated<br>Spent Fuel Plus Basalt (AP-83)



TIME (hours)



Effect of Temperature on Sodium and Silicon Concentrations for<br>Simulated Spent Fuel Plus Basalt (AP-83)



Figure 6.5-4

# Effect of Temperature on Chloride and Sulfate Concentrations<br>for Spent Fuel Plus Basalt (AP-83)



Figure  $6.5-5$ 





TIME (hours)



Effect of Temperatures on Strontium and Uranium Concentrations<br>for Simulated Spent Fuel Plus Basalt (AP-83)



TIME (hours)

# Figure 6.5-7

Effect of Temperature on Cesium and Molybdenum<br>Concentrations for Simulated Spent Fuel Plus<br>Basalt (AP-83)

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# APPENDIX A

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## Will be Obtained from NRC

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