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THERMAL ANALYSIS OF THE NATIONAL
RADIOACTIVE WASTE REPOSITORY:
PROGRESS THROUGH JUNE 1971

R. D. Cheverton
W. D. Turner

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CHEMICAL TECHNOLOGY DIVISION

THERMAL ANALYSIS OF THE NATIONAL RADIOACTIVE
WASTE REPOSITORY: PROGRESS THROUGH JUNE 1971

R. D. Cheverton
W. D. Turner*

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DECEMBER 1971

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THERMAL ANALYSIS OF THE NATIONAL RADIOACTIVE
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ABSTRACT

Solidified high-level fuel reprocessing wastes and alpha-contaminated solid wastes are to be placed in salt formations 1000 ft below the earth's surface at the proposed National Radioactive Waste Repository near Lyons, Kansas. The heat released from these wastes will result in temperature increases throughout the immediate geologic formations. The following several factors influence the permissible temperature rises: (1) thermal instability of the solidified waste; (2) migration of brine; (3) integrity of the mine during operation; (4) integrity of the overlying formations; (5) temperature in freshwater aquifers; (6) temperature of the earth's surface; and (7) temperatures beyond the boundaries of the mine. Preliminary thermal calculations indicated the technical feasibility of the Repository. More recent analyses have considered the Repository in greater detail and have employed updated thermal property and stratigraphic data. The results from these analyses indicate that all of the criteria can be satisfied, and that a heat load of about 130 kW/acre is acceptable for 10-year-old high-level waste.

1. INTRODUCTION

One consequence of generating power with nuclear fission energy is the creation of radioactive wastes. The most important types of such wastes are: (1) concentrated fission products, which are intense sources of gamma radiation and are referred to as high-level waste; and (2) alpha wastes, which are composed of miscellaneous materials that have been contaminated during fuel fabrication and reprocessing and other operations with alpha emitters such as plutonium and its daughter products. Both of these types of waste must be disposed of in a way that will not result in contamination of the biosphere during the thousands of years required for the radioactivity to decay to a harmless level.

The Atomic Energy Commission, in consultation with the National Academy of Sciences and members of the geologic community, has tentatively concluded

that permanent disposal of radioactive wastes can be achieved most effectively through burial of the wastes in salt deposits, after the waste has been concentrated and solidified. This scheme appears to be basically sound because salt deposits are normally free of circulating groundwaters, are protected from underground aquifers by virtually impermeable shale, and, due to their plastic deformation and recrystallization characteristics, are self-healing in the event that a fracture occurs. Furthermore, salt appears to have adequate structural and thermal properties, is abundant, is easily mined, and is generally located in zones of low seismicity.

An important characteristic of radioactive waste that must be considered in connection with waste handling and storage is heat generation. The heat is generated in the waste as a result of radioactive decay. After the waste is buried in the mine, the heat is dissipated in the salt and surrounding formations and eventually flows to the surface of the earth, where it is transferred to the atmosphere and flowing groundwater. A consequence of the subsurface heat release is an increase in the temperatures of the mined area and its environs. These temperatures gradually increase at first, and then finally decrease since the heat generation rate in the waste is continuously decreasing. Eventually the heat source will decay completely, and the temperatures will return to normal; however, the time scale is thousands of years.

During the period of significant heat release, temperature limitations must be considered to ensure mine operability and absolute confinement of the waste. Factors that influence the allowable heat release rate include: (1) thermal instability of the solidified waste; (2) release and migration of brine contained in small cavities in the salt; (3) structural integrity of the mine during operation; (4) structural integrity of the entire formation; (5) temperature rise in freshwater aquifers; (6) heating of the earth's surface; and (7) temperature increases beyond the boundaries of the mine.

Detailed thermal and rock mechanics design studies associated with waste solidification and burial have been in progress since the latter part of 1968. These studies are based on the concept that the high-level solidified waste would be enclosed in stainless steel containers several

inches in diameter and several feet long. This package (i.e., the contained waste) would then be placed in a vertical hole in the salt beneath the floor of a room mined out of the salt formation. Many such packages would be placed beneath a room, and the holes and the room would be back-filled with crushed salt. The room, pillar and package dimensions, the number of packages per room, and the power per package would be optimized for safety and economics. The alpha waste would be placed in crates and/or drums, which, in turn, would be placed in rooms that later would be backfilled with crushed salt.

The particular salt deposit selected for waste burial is near Lyons, Kansas, where a salt mine was once operated. It is intended that the alpha waste be placed in existing rooms in the mine, and that new, customized rooms be prepared for receiving the high-level waste.

Thermal studies prior to January 1971 were conducted by R. L. Bradshaw and J. J. Perona.¹ The results of these studies, coupled with rock mechanics analyses performed by W. C. McClain,¹ indicated that the waste burial scheme was feasible. However, the studies, which of necessity covered a broad range of variables, were considered to be only a preliminary effort. It was recognized that improvements in modeling and more accurate materials property data were required, and that a higher degree of optimization was desirable.

Since January 1971 the emphasis has been centered on improving the thermal calculational models and the numerical analysis techniques; on obtaining more representative thermal property data and more accurate stratigraphic detail; and on obtaining a consistent set of time-dependent waste and geologic formation temperatures for specific, yet typical, room, pillar, and waste-package arrangements. Sensitivity studies have also been conducted to evaluate the importance of the uncertainties that remain. The progress made with regard to this effort through June 1971 is the subject of this report.

In addition to the radioactive decay heat release mechanism, there is, in principle, a mechanism for sudden release of stored energy. Energy is stored in the solidified waste and surrounding salt as a result of

radiation damage, and the release of this energy may be triggered by an increase in temperature. Hypothetical transients following such a release last about one day, with temperatures reaching a maximum and returning to normal within that time. Details of the mechanism and calculations are reported elsewhere.²

2. SOLUTION OF THE HEAT CONDUCTION DIFFERENTIAL EQUATION

Heat is transferred from the waste package and throughout the surrounding geologic formation primarily by conduction. Some radiation and natural convection will occur in voids adjacent to the waste package and in the partially backfilled rooms. Heat will also be transferred by convection to the aquifers, which are located within 300 ft of the earth's surface, and via convection and radiation from the earth's surface to the atmosphere and to space. The nature of the problem at hand is such that the contributions from radiation and convection are small insofar as their effects on pertinent temperatures are concerned. An exception is in the calculation of the temperature of a flowing aquifer; however, this can be treated as a separate analysis. Thus the basic problem associated with heat removal from the buried waste is one of conduction.

The differential heat conduction equation is:

$$C_p \rho \frac{\partial T}{\partial t} = Q + \nabla(k \nabla T) , \quad (2.1)$$

where

T = temperature,

t = time,

Q = heat generation rate per unit volume,

C_p = specific heat,

ρ = density,

k = thermal conductivity.

Analytical solutions can be obtained to Eq. (2.1) only for simplified calculational models. Since the Waste Repository constitutes a relatively complex problem, one must resort to numerical solutions and large computers. This approach introduces questions regarding accuracy and makes selection

of appropriate numerical methods quite important. Monte Carlo, hybrid (analog-digital), finite element, and finite difference are some of the methods that have been considered. The last method is presently being applied to the one-, two-, and three-dimensional conduction equations for the Repository. It has been under development for a longer period of time and has been much more widely used than the others.

There are many finite difference techniques for obtaining solutions to the heat conduction equation. The basic differences between them are associated primarily with the selection of the effective temperature or temperature change during a finite time step. These and other, related differences affect the accuracy and the economy associated with a specific problem. Thus it is of some interest to compare some of the more highly developed techniques. As a matter of convenience, a two-dimensional problem will be considered in which the heat generation term is zero, and the material thermal conductivity (k), specific heat (C_p), and density (ρ) are independent of position and temperature. The boundary value problem of interest becomes:

$$\begin{aligned} U_t &= U_{xx} + U_{yy}, \quad (x,y) \in R, \quad 0 < t \leq t_f \\ U(x,y,0) &= f(x,y), \quad (x,y) \in R \\ U(x,y,t) &= g(x,y,t), \quad (x,y) \in \partial R, \quad 0 < t \leq t_f, \end{aligned} \quad (2.2)$$

where

R is the unit square and ∂R is its boundary.

A finite difference approximation to U_{xx} and U_{yy} at point (x_i, y_j) for equal mesh spacings is:

$$\begin{aligned} U_{xx} &= \frac{W_{i-1,j} - 2W_{i,j} + W_{i+1,j}}{a^2} \\ U_{yy} &= \frac{W_{i,j-1} - 2W_{i,j} + W_{i,j+1}}{b^2}, \end{aligned} \quad (2.3)$$

where

$$w_{ij}^n = U(x_i, y_j, t_n), \quad (2.4)$$

$$a = \Delta x = 1/N_x,$$

$$b = \Delta y = 1/N_y,$$

$$\left. \begin{aligned} x_i &= ia, & 0 \leq i \leq N_x \\ y_j &= jb, & 0 \leq j \leq N_y \\ t_n &= n\Delta t, & 0 \leq n \end{aligned} \right\} \begin{array}{l} i, j, \text{ and } n \text{ are integers} \end{array}$$

Δt = time step.

The finite difference approximation for U_t is simply $\frac{\Delta T_i}{\Delta \tau}$, where ΔT_i is the change in temperature at node i corresponding to a time increment $\Delta \tau$. The various finite difference techniques consider $\Delta \tau$ values that are not necessarily equal to Δt . Furthermore, each of the terms on the right-hand side of Eq. (2.3) can correspond to different times [this is why specific times are not indicated in Eq. (2.3)].

The initial condition for the above general finite difference equation is:

$$w_{ij}^0 = f_{ij}, \quad 0 \leq i \leq N_x, \quad 0 \leq j \leq N_y, \quad (2.5)$$

and the boundary conditions are represented by:

$$w_{ij}^n = g_{ij}^n, \quad (ia, jb) \in \partial R, \quad n > 0. \quad (2.6)$$

The transient temperatures in R can be calculated by using Eqs. (2.5) and (2.6) and one of the techniques mentioned below.

2.1 Discussion of Specific Techniques

In the following presentation of equations, it is convenient to make use of the following operators [refer to Eq. (2.3)]:

$$\begin{aligned} \Delta_x^2 f_{ij} &= \frac{f_{i-1,j} - 2f_{i,j} + f_{i+1,j}}{a^2} \\ \Delta_y^2 f_{ij} &= \frac{f_{i,j-1} - 2f_{i,j} + f_{i,j+1}}{b^2}. \end{aligned} \quad (2.7)$$

2.1.1 The Classical Explicit Procedure (CEP)

The Classical Explicit Procedure is represented by

$$\frac{W_{ij}^{n+1} - W_{ij}^n}{\Delta t} = \Delta_x^2 W_{ij}^n + \Delta_y^2 W_{ij}^n . \quad (2.8)$$

It has an error of

$$e = O(a^2) + O(b^2) + O(\Delta t) , \quad (2.9)$$

where $e = O[f(x)]$ implies $|e| \leq Af(x)$ as x approaches some limit. The CEP technique is stable if the time increment satisfies³⁻⁵

$$\Delta t \leq \frac{1}{2} (a^{-2} + b^{-2})^{-1} . \quad (2.10)$$

It is easy to use, requires the least amount of operations per time step, and is probably the most reliable technique at the present time for general heat transfer problems in which unequal mesh spacing, irregular boundaries, temperature- or time-dependent parameters, and nonlinear boundary conditions are requisites. Hence, it is widely used.⁶⁻¹² For problems requiring small mesh increments, the time step must be small to ensure stability. This makes a large number of time steps necessary and, in turn, requires a large amount of computation to calculate the transient temperature distribution for long periods of time. Modifications to the basic explicit scheme have been developed by Levy,^{13,14} by Winson,¹⁵ and by Barakat and Clark.¹⁶ These modifications remove the stability criterion in Eq. (2.10). Levy's method differences the time derivative at point (i,j) by

$$\left. \frac{\partial U}{\partial t} \right|_{(i,j)} = \frac{(1+Z_{ij})(W_{ij}^{n+1} - W_{ij}^n) - Z_{ij}(W_{ij}^n - W_{ij}^{n-1})}{\Delta t} , \quad (2.11)$$

where

$$Z_{ij} = \begin{cases} 0, & \text{if } D_{ij} \leq 1 \\ \frac{D_{ij} - 1}{2}, & \text{if } D_{ij} > 1 \end{cases} \quad (2.11a)$$

and

$$D_{ij} = 2\Delta t(a^{-2} + b^{-2}) . \quad (2.11b)$$

For a time increment of given size, the Levy-modified CEP is not as accurate as the basic CEP;¹⁷ however, its accuracy is sufficient to permit much larger time steps than are used in the basic CEP technique. In some of the three-dimensional analyses of the Repository, a factor of 50 on the time step has been used.

2.1.2 The Classical Implicit Procedure (CIP)

The Classical Implicit Procedure is described by:

$$\frac{w_{ij}^{n+1} - w_{ij}^n}{\Delta t} = \Delta_x^2 w_{ij}^{n+1} + \Delta_y^2 w_{ij}^{n+1} . \quad (2.12)$$

It has an error given by Eq. (2.9) and is unconditionally stable.^{3,5} The CIP has been used by a number of individuals throughout various industrial fields.^{12,18} However, for two- and three-dimensional problems, its use requires the solution of a large set of simultaneous equations at each time step; thus the amount of computation required per time step is considerably greater than for the CEP.

2.1.3 The Crank-Nicolson Implicit Scheme (CN)

The Crank-Nicolson Implicit Scheme is represented by:

$$\frac{w_{ij}^{n+1} - w_{ij}^n}{\Delta t} = \frac{1}{2} \Delta_x^2 (w_{ij}^n + w_{ij}^{n+1}) + \frac{1}{2} \Delta_y^2 (w_{ij}^n + w_{ij}^{n+1}) . \quad (2.13)$$

It has an error of

$$e = O(a^2) + O(b^2) + O(\Delta t^2) , \quad (2.14)$$

and it, too, is unconditionally stable.^{3,5,19} Since this technique is more accurate with respect to time than either the CEP or the CIP, it represents an improved means for solving problems such as Eq. (2.2). However, for two- and three-dimensional problems, its use requires the solution of a large set of simultaneous, linear algebraic equations at each time step.

2.1.4 The Peaceman-Rachford Alternating Direction Implicit (ADI) Method

The Peaceman-Rachford Alternating Direction Implicit Method is represented by:

$$\begin{aligned} \frac{w_{ij}^{*n+1} - w_{ij}^n}{\Delta t} &= \frac{1}{2} \Delta_x^2 (w_{ij}^n + w_{ij}^{*n+1}) + \Delta_y^2 w_{ij}^n \\ \frac{w_{ij}^{n+1} - w_{ij}^{*n+1}}{\Delta t} &= \frac{1}{2} \Delta_x^2 (w_{ij}^{*n+1} + w_{ij}^{n+1}) + \frac{1}{2} \Delta_y^2 (w_{ij}^n + w_{ij}^{n+1}). \end{aligned} \quad (2.15)$$

It has an error given by Eq. (2.14) and is unconditionally stable.^{3,5,20} The system of linear equations arising from the finite difference approximation is tridiagonal and, hence, can be solved efficiently by means of a special form of Gaussian elimination.²⁰ Thus, the ADI method is one of the most economical methods for solving Eq. (2.2). Peaceman and Rachford showed that the CEP and the CIP required about 25 times and 7 times, respectively, more computation than the ADI to solve a problem similar to Eq. (2.2).²⁰

An extension of the Peaceman-Rachford method to the solution of three-dimensional problems is found in ref. 21, and an improved version of the method is described in ref. 22. Other ADI schemes that have been developed are described in refs. 21-27.

2.1.5 The Alternating Direction Explicit Method (ADE)

The Alternating Direction Explicit Method was first introduced by Saul'ev²⁸ and was later extended by Larkin.^{29,30} It is described by:

$$\begin{aligned} \frac{w_{ij}^{n+1} - w_{ij}^n}{\Delta t} &= \frac{w_{i-1,j}^{n+1} - (w_{ij}^{n+1} + w_{ij}^n) + w_{i+1,j}^n}{a^2} \\ &+ \frac{w_{i,j-1}^{n+1} - (w_{ij}^{n+1} + w_{ij}^n) + w_{i,j+1}^n}{b^2} \end{aligned} \quad (2.16)$$

for increasing i and j , and by

$$\frac{w_{ij}^{n+2} - w_{ij}^{n+1}}{\Delta t} = \frac{w_{i-1,j}^{n+1} - (w_{ij}^{n+1} + w_{ij}^{n+2}) + w_{i+1,j}^{n+2}}{a^2} + \frac{w_{i,j-1}^{n+1} - (w_{ij}^{n+1} + w_{ij}^{n+2}) + w_{i,j+1}^{n+2}}{b^2}$$

for decreasing i and j .

This method is another example of explicit techniques that are unconditionally stable.²⁸⁻³⁰ Initially it was thought that the accuracy of the ADI and the accuracy of the ADE method were comparable, and that the ADE method required considerably less computation than the ADI method to calculate the transient temperature distribution to a specific time.^{30,31} Recently, however, some doubt has been cast on the accuracy of the ADE techniques; furthermore the techniques are not as fast as was first believed.³²

2.1.6 Selection of Techniques for the Repository

Equal mesh spacings, equal time increments, and space-independent thermal properties were assumed, as indicated by Eq. (2.2), in the preceding comparative evaluation of the various finite difference techniques. Most of the physical problems considered for the Repository are much more complicated than this. For example, many different materials are usually present in irregular patterns. In order to accurately represent the details using a finite difference technique, the use of unequal mesh spacing along each axis is necessary. Also, the boundaries are no longer rectangular. Some questions have been raised regarding the stability of implicit techniques³³⁻³⁷ for problems with irregular boundaries, unequal mesh spacing, and temperature- and time-dependent parameters; thus they must be used with caution. Awareness of this situation plus the proven stability of the CEP technique has led to more extensive use of this method at ORNL in connection with the Waste Repository. However, the complexity and the number of the calculations that must be made for the Repository are increasing to the point where a faster, yet sufficiently accurate, technique must be developed. The ADI technique is presently

being applied to a few special problems for the purpose of investigating stability characteristics and accuracy. The ORNL CEP and ADI techniques are discussed below.

2.1.7 The ORNL CEP Technique

The ORNL CEP technique is incorporated in the HEATING^{6,38} code. This code is capable of solving parabolic differential equations in one, two, and three dimensions for Cartesian and cylindrical coordinates. The finite difference heat balance equation for node o is:

$$C_o \frac{T_o^{n+1} - T_o^n}{\Delta t} = P_o^n + \sum_{m=1}^6 K_m (T_m^n - T_o^n) , \quad (2.17)$$

where T_m^n is the temperature of the m th node adjacent to node o at time $n\Delta t$, K_m is the conductance between nodes o and m, C_o is the heat capacitance of the material associated with node o, and P_o is the power generation in the latter material. Since mesh lines go through the nodes, as many as eight different materials can touch a node and four different materials can be positioned (in parallel) between adjacent nodes. For a three-dimensional problem, an interior node will have, at any particular time, $n\Delta t$, one C, one P, and six K's. These parameters are calculated as follows for node o:

$$C_o = \sum_{l=1}^8 C_{pl} \rho_l V_l , \quad (2.18)$$

$$P_o^n = \sum_{l=1}^8 q_l^n V_l , \quad (2.19)$$

$$K_m = \frac{1}{L_E} \sum_{\gamma=1}^4 k_{m\gamma} A_{m\gamma} , \quad (2.20)$$

where

C_{pl} = specific heat for region l ,

ρ_l = density for region l ,

V_l = volume of region l ,

Q_l^n = power density in region l at time $n\Delta t$,

K_m = conductance between node o and adjacent node m ,

L_m = distance between node o and adjacent node m ,

k_{my} = thermal conductivity for region y between nodes o and m ,

A_{my} = cross-sectional area, normal to heat flow path, of region y between nodes o and m .

With reference to Fig. 2.1, the V_l 's and A_{my} 's are further defined, by using examples, as follows:

$$V_1 = \frac{(X_{i+1} - X_i)}{2} \frac{(Y_{j+1} - Y_j)}{2} \frac{(Z_{k+1} - Z_k)}{2} \quad (2.21)$$

$$A_{1,1} = \frac{(Y_{j+1} - Y_j)}{2} \frac{(Z_{k+1} - Z_k)}{2} \quad (2.22)$$

Equation (2.17) can be readily solved for T_o^{n+1} to give:

$$T_o^{n+1} = T_o^n + \frac{\Delta t}{C_o} \left[P_o^n + \sum_{m=1}^6 K_m (T_m^n - T_o^n) \right] \quad (2.23)$$

The numerical solution obtained by using this equation is stable, provided the following equation is satisfied:

$$\Delta t \leq \left(\frac{C_o}{6 \sum_{m=1}^6 K_m} \right) \quad (2.24)$$

minimum for all nodes

Fig. 2.1. Nodal Description for Three-Dimensional Problem.

The restriction imposed by Eq. (2.24) is excessive in terms of computer time for many problems encountered in connection with the analysis of the Repository. Thus, Levy's modification (Sect. 2.1.1) has been incorporated in HEATING and has been used for the solution of several two- and three-dimensional problems.

2.1.8 The ORNL ADI Technique

A new code has recently been developed at ORNL for solving the three-dimensional, transient heat conduction equation in Cartesian coordinates, using the ADI technique proposed by Douglas.²² This technique uses three equations similar to Eq. (2.17) to calculate the temperature for node o at time $t + \Delta t$. For the first equation, Eq. (2.17) is written implicitly with respect to the nodes along the X-axis, and explicitly with respect to the nodes along the Y- and Z-axes. For the second equation, Eq. (2.17) is written implicitly with respect to the nodes along the Y-axis; for the third equation, it is written implicitly with respect to the nodes along the Z-axis. The three equations may be written as:

$$C_o \frac{T_o^{*n+1} - T_o^n}{\Delta t} = P_o^{n+1/2} + \sum_{m=1}^2 K_m \left[\frac{T_m^{*n+1} + T_m^n}{2} - \frac{T_o^{*n+1} + T_o^n}{2} \right] + \sum_{m=3}^6 K_m (T_m^n - T_o^n), \quad (2.25a)$$

$$C_o \frac{T_o^{**n+1} - T_o^n}{\Delta t} = P_o^{n+1/2} + \sum_{m=1}^2 K_m \left[\frac{T_m^{*n+1} + T_m^n}{2} - \frac{T_o^{*n+1} + T_o^n}{2} \right] + \sum_{m=3}^4 K_m \left[\frac{T_m^{**n} + T_m^n}{2} - \frac{T_o^{**n+1} + T_o^n}{2} \right] + \sum_{m=5}^6 K_m (T_m^n - T_o^n), \quad (2.25b)$$

$$\begin{aligned}
C_o \frac{T_o^{n+1} - T_o^n}{\Delta t} = & P_o^{n+1}/2 + \sum_{m=1}^2 K_m \left[\frac{T_m^{*n+1} + T_m^n}{2} - \frac{T_o^{*n+1} + T_o^n}{2} \right] \\
& + \sum_{m=3}^4 K_m \left[\frac{T_m^{**n+1} + T_m^n}{2} - \frac{T_o^{**n+1} + T_o^n}{2} \right] \\
& + \sum_{m=5}^6 K_m \left[\frac{T_m^{n+1} + T_m^n}{2} - \frac{T_o^{n+1} + T_o^n}{2} \right], \quad (2.25c)
\end{aligned}$$

where T^{*n+1} and T^{**n+1} are the first and second estimates, respectively, of the temperature of a particular node at $t + \Delta t$. T_o , C_o , P_o , and K_m are defined as in Sect. 2.1.7.

In effect, the problem is first solved for each time step with Eq. (2.25a) to obtain the $T_m^{*(n+1)}$ temperatures. Using these temperatures and Eq. (2.25b), the problem is solved again, this time for the $T_m^{**(n+1)}$ temperatures. Finally, Eq. (2.25c) is used to solve for the T_m^{n+1} temperatures. Each of the three equations results in a tridiagonal system of equations that can be solved very efficiently.²⁰

3. MODELING THE REPOSITORY

The particular modeling that must be considered for the thermal analysis of the Waste Repository depends upon the specific thermal criteria and upon thermal input requirements for the structural and flow analysis of the geologic formation. Presumably, the degree of sophistication will increase as the overall analysis of the Repository progresses. It is possible that a three-dimensional analysis (directly or by synthesis) of the entire Repository, including some detail in the rooms, will have to be performed. However, at the present time, it appears that a considerable amount of symmetry can be assumed for the bulk of the calculations without jeopardizing the intent of the analysis, which, at this point, is to demonstrate technical feasibility.

3.1 Selection of Models

The thermal data requirements, as they pertain to the selection of a particular model, will be reviewed before the details of the most extensively used models are discussed. Criteria based on the earlier studies of Bradshaw and McClain¹ specify limits on salt temperatures in the vicinity of the waste container and in the pillar. The concepts upon which these criteria are based are discussed elsewhere. It is sufficient here to state that they are of the "maximum permissible" type without particular regard to histories and space and time gradients. Therefore, it is possible to consider a "worst" case that will result in conservatively high temperatures. For the particular case being considered, this allows the use of symmetry; however, because of the detailed nature of the problem (temperatures in and close to the waste container and pillar), a three-dimensional (3-D) model is required. One of the typical 3-D models for the high-level waste is illustrated in Fig. 3.1. As indicated, planes of symmetry are placed at the vertical center lines of the room and the pillar, at a point midway between the waste containers, and through the vertical center line of the waste container. In effect, the mine is infinite in horizontal extent, with infinitely long rooms containing identical wastes.

Fig. 3.1. Three-Dimensional Model of a Unit Cell of the High-Level Mine.

Specific criteria per se do not exist in connection with the detailed structural and flow analysis of the geologic formation, although temperature distributions throughout the Repository are required as input to the analysis. This type of information can be obtained by synthesizing results for a two-dimensional (RZ) [2-D (RZ)] and a 3-D or a two-dimensional (XZ) [2-D (XZ)] model, and in some cases by using the 2-D (RZ) model alone. Typical 2-D (XZ) and 2-D (RZ) models being used at this time for the high-level waste are illustrated in Figs. 3.2 and 3.3 respectively. As indicated in Fig. 3.2, the 2-D (XZ) model simulates the 3-D room and pillar model (Fig. 3.1), using a vertical plane or slab source. The 2-D (RZ) model (Fig. 3.3) covers the entire Repository from well below the mine area to the earth's surface and radially to a point well beyond the edge of the mined area. The source "zone" is represented by a disc or concentric annuli, depending on whether the waste loading is treated as instantaneous or sequential. In either case, symmetry is assumed about the vertical center line of the Repository.

Although they are very loosely defined at this time, criteria exist for the heat flux at the earth's surface, for aquifer temperature increases, and for "mineral" temperatures beyond the Repository. The 2-D (RZ) model appears to be satisfactory for predicting conservative temperature increases in these areas.

With regard to the notion that "conservative" calculations can be performed, it is important that information pertaining to the geologic formations and their thermal properties be reasonably accurate and that they be properly included in the models. For instance, a maximum-power-density unit cell model will not necessarily yield maximum temperatures if adjacent maximum-power-density unit cells have a much thicker shale layer overhead. The major problem in this regard is obtaining the basic geologic and thermal property data over the entire Repository. As an alternative to having all the data, somewhat arbitrary perturbations are being imposed on the nominal conditions to obtain degrees of sensitivity. The detailed models described below reflect this effort to some extent.

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Fig. 3.2. Two-Dimensional XZ Model of a Unit Cell of the High-Level Mine.

ORNL DWG 71-2901

Fig. 3.3. Two-Dimensional Cylindrical Model of the High-Level Mine.

3.2 Details of the 3-D and 2-D Models

3.2.1 Three-Dimensional Model

The basic 3-D models for the high-level portion of the Repository are shown in Figs. 3.1, 3.4, and 3.5 for 30-, 50-, and 15-ft-wide rooms respectively. The dimensions of the region, the composition and thermal properties of the materials, and the mesh spacing for typical cases are shown in Tables 3.1-3.3. It is observed that the vertical height is confined within $Z = 600$ and 1400 ft rather than extending all the way to the surface and far below the mine. Also, these two boundaries have fixed temperatures in the calculations. These approximations are permitted because only the first 50 years of mine operation are considered (local temperatures reach a maximum within this period of time); at the end of this time, temperature changes at these boundaries are very small. This condition was determined from 2-D calculations that included increased and decreased heights and from 3-D calculations that included a decreased height.

The mesh spacings and dimensions of the region in the 3-D models are sufficiently small that temperatures can be calculated up to the surface of the waste container. Temperature profiles within the waste container are calculated with a steady-state analytical solution.

3.2.2 Two-Dimensional (XZ) Model

A 2-D (XZ) model is used to study the effects of variations in the stratigraphy within the high-level mine area and to obtain longer-term temperature data in this area. A typical model is illustrated in Fig. 3.2 for a 30-ft room; other related data are provided in Table 3.4. In this particular model, the waste containers are smeared throughout a vertical, infinitely-long slab that has the height and thickness of the waste container. Temperatures obtained from this model are essentially the same as those obtained from the above 3-D model up to a position a few feet from the waste container. For operating times longer than 50 years, the upper and lower boundaries are extended as necessary.

ORNL-DWG-71-9503

Fig. 3.4. Three-Dimensional Model of a Unit Cell of the High-Level Mine - 50-ft Room.

ORNL-DWG-71-9511

Fig. 3.5. Three-Dimensional Model of a Unit Cell of the High-Level Mine - 15-ft Room.

Table 3.1. Description of Three-Dimensional Model
for a 30-ft Room in the Repository

(Also refer to Fig. 3.1)

A. Region Definition

Region No.	Material No.	Left x^a	Right x^a	Front y^a	Back y^a	Top z^a	Bottom z^a
1	5	0	30	0	11	600	800
2	3	0	30	0	11	800	900
3	2	0	30	0	11	900	985
4	1	0	30	0	11	1025	1050
5	5	0	30	0	11	1050	1400
6	4	0	15	0	11	990	1000
7	1	15	30	0	11	985	1000
8	1	0	30	0	11	1000	1002
9	5	0	30	0	11	1002	1004
10	1	0	30	0	11	1004	1008
11	1	0	30	0	11	1018	1021
12	5	0	30	0	11	1021	1025
13	1	0	10.75	0	0.25	1008	1018
14 ^b	6	10.75	11.25	0	0.25	1008	1018
15	1	11.25	30	0	0.25	1008	1018
16	1	0	30	0.25	11	1008	1018

B. Description and Properties of Material

Material No.	Description	k [Btu hr ⁻¹ ft ⁻¹ (°F) ⁻¹]	ρ (lb/ft ³)	C_p [Btu lb ⁻¹ (°F) ⁻¹]
1	Salt	1.81	135	0.22
2	80% salt, 20% shale	1.32	138	0.216
3	50% salt, 50% shale	1.01	142.5	0.21
4	Crushed salt	0.13	98	0.21
5	Shale	0.635	150	0.20
6	Calcine	0.250	113	0.22

C. Nodal Point Locations

Node	x^a	y^a	z^a
1	0	0	600
2	3	0.25	700
3	6	0.75	800
4	8	1.5	900
5	9.5	3.0	950
6	10.25	5.0	980
7	10.75	8.0	985
8	11.25	11.0	990
9	11.75		995
10	12.5		1000
11	14		1002
12	17		1004
13	17		1006
14	20		1008
15	25		1010.5
16	30		1013
17			1015.5
18			1018
19			1021
20			1025
21			1050
22			1100
23			1200
24			1300
25			1400

^aDimensions are given in ft.

^bHeat generation occurs in this region.

Table 3.2. Description of Three-Dimensional Model
for a 50-ft Room in the Repository
(Also refer to Fig. 3.4)

A. Region Definition

Region No.	Material No.	Left x^a	Right x^a	Front y^a	Back y^a	Top z^a	Bottom z^a
1	6	0	50	0	21	600	800
2	5	0	50	0	21	1002	1004
3	6	0	50	0	21	1021	1025
4	6	0	50	0	21	1050	1400
5	4	0	50	0	21	800	900
6	3	0	50	0	21	900	985
7	5	0	25	0	21	990	1000
8	2	25	50	0	21	985	1000
9	2	0	50	0	21	1000	1002
10	2	0	16	0	21	1004	1021
11	2	16	25	5	21	1004	1021
12	2	25	50	0	21	1004	1021
13	2	0	50	0	21	1025	1050
14	1	16	20.75	0	5	1004	1021
15	1	20.75	21.25	0.25	5	1004	1021
16	1	21.25	25	0	5	1004	1021
17	1	20.75	21.25	0	0.25	1004	1008
18	1	20.75	21.25	0	0.25	1018	1021
19b	7	20.75	21.25	0	0.25	1008	1018

B. Description and Properties of Material

Material No.	Description	k [Btu hr ⁻¹ ft ⁻¹ (°F) ⁻¹]	ρ (lb/ft ³)	C_p [Btu lb ⁻¹ (°F) ⁻¹]
1	Salt, 462°F	1.6	135.0	0.220
2	Salt, 592°F	1.8	135.0	0.220
3	80% salt, 20% shale	1.53	138.0	0.216
4	50% salt, 50% shale	1.37	142.5	0.210
5	Crushed salt	0.13	98.0	0.210
6	Shale	0.952	150.0	0.200
7	Calcine	0.25	113.0	0.220

C. Nodal Point Locations

Node	x^a	y^a	z^a
1	0	0	600
2	5	0.25	700
3	10	0.75	800
4	13	1.5	900
5	16	3	950
6	18	5	980
7	19.5	8	985
8	20.25	11	990
9	20.75	16	995
10	21.25	21	1000
11	21.75		1002
12	22.5		1004
13	24		1006
14	25		1008
15	27		1010.5
16	30		1013
17	35		1015.5
18	40		1018
19	45		1021
20	50		1025
21			1050
22			1100
23			1200
24			1300
25			1400

^aDimensions are given in ft.

^bHeat generation occurs in this region.

Table 3.3. Description of Three-Dimensional Model
for a 15-ft Room in the Repository

(Also refer to Fig. 3.5).

A. Region Definition

Region No.	Material No.	Left x^a	Right x^a	Front y^a	Back y^a	Top z^a	Bottom z^a
1	6	0	20	0	21	600	800
2	6	0	20	0	21	1000	1004
3	6	0	20	0	21	1021	1025
4	6	0	20	0	21	1050	1400
5	4	0	20	0	21	900	900
6	3	0	20	0	21	900	985
7	5	0	7.5	0	21	990	1000
8	2	7.5	20	0	21	985	1000
9	2	0	20	0	21	1000	1002
10	2	0	5	5	21	1004	1021
11	2	5	20	0	21	1004	1021
12	2	0	20	0	21	1025	1050
13	1	0	0.25	0	0.25	1004	1008
14	1	0	0.25	0	0.25	1018	1021
15	1	0	0.25	0.25	5	1004	1021
16	1	0.25	5	0	5	1004	1021
17 ^b	7	0	0.25	0	0.25	1008	1018

B. Description and Properties of Material

Material No.	Description	k [Btu hr ⁻¹ ft ⁻¹ (°F) ⁻¹]	ρ (lb/ft ³)	C_p [Btu lb ⁻¹ (°F) ⁻¹]
1	Salt, 482°F	1.6	135.0	0.220
2	Salt, 392°F	1.8	135.0	0.220
3	80% salt, 20% shale	1.53	138.0	0.216
4	50% salt, 50% shale	1.37	142.5	0.210
5	Crushed salt	0.13	98.0	0.210
6	Shale	0.952	150.0	0.200
7	Calcine	0.25	113.0	0.220

C. Nodal Point Locations

Node	x^a	y^a	z^a
1	0	0	600
2	0.25	0.25	700
3	0.75	0.75	800
4	1.5	1.5	900
5	3	3	950
6	5	5	980
7	7.5	8	985
8	10	11	990
9	15	16	995
10	20	21	1000
11			1002
12			1004
13			1006
14			1008
15			1010.5
16			1013
17			1015.5
18			1018
19			1021
20			1025
21			1050
22			1100
23			1200
24			1300
25			1400

^aDimensions are given in ft.^bHeat generation occurs in this region.

Table 3.4. Description of Two-Dimensional Rectangular Model
for a 30-ft Room in the Repository

(Also refer to Fig. 3.2)

A. Region Definition

Region No.	Material No.	Left X^a	Right X^a	Upper Z^a	Lower Z^a
1	5	0	30	700	800
2	3	0	30	800	900
3	2	0	30	900	985
4	1	0	30	1025	1050
5	5	0	30	1050	1300
6	4	0	15	990	1000
7	1	15	30	985	1000
8	1	0	30	1000	1002
9	5	0	30	1002	1004
10	1	0	30	1004	1008
11	1	0	30	1018	1021
12	5	0	30	1021	1025
13	1	0	30	1008	1018

B. Description and Properties of Materials

Material No.	Description	k [Btu hr ⁻¹ ft ⁻¹ (°F) ⁻¹]	ρ (lb/ft ³)	C_p [Btu lb ⁻¹ (°F) ⁻¹]
1	Salt	1.81	135	0.22
2	80% salt, 20% shale	1.32	138	0.216
3	50% salt, 50% shale	1.01	142.5	0.21
4	Crushed salt	0.13	98	0.21
5	Shale	0.635	150	0.20

C. Nodal Point Locations

Node	X^a	Z^a
1	0	700
2	3	800
3	6	900
4	9	950
5	11	980
6	13	985
7	15	990
8	17	995
9	20	1000
10	25	1002
11	30	1004
12		1006
13		1008
14		1010.5
15		1013
16		1015.5
17		1018
18		1021
19		1025
20		1050
21		1100
22		1200
23		1300

^aDimensions are given in ft.

Note: Heat generation is effectively located in the area bounded by
 $X = 10$, $X = 12$, $Z = 1007$ to $Z = 10019.5$.

3.2.3 Two-Dimensional (RZ) Model

The 2-D (RZ) model for the high-level waste is illustrated in Fig. 3.3; typical supplementary data are given in Table 3.5. As indicated, this model considers the entire Repository, extending from the earth's surface to 2500 ft below the room floor level (1000 ft) and radially to 3000 ft beyond the edge of the mine. The waste is considered to be smeared throughout a disc 20 ft thick and 7000 ft in diameter (~880 acres). This disc can contain several annular regions, each with a different heat source. Although the annular array does not simulate the geometry or sequencing for an actual expanding-mine problem, it has been useful for evaluating the effects of time-dependent loadings.

The same 2-D (RZ) model was used for the alpha-mine studies, with the exception that the disc source was only 3200 ft in diameter (~180 acres) and 10 ft thick.

3.3 Boundary Conditions

The boundary conditions are specified and discussed above. However, a comment regarding the fixed-temperature boundary at the earth's surface is in order. The earth's surface temperature will, of course, increase to some extent. The increase is estimated by means of a radiation heat transfer analysis, using the surface heat flux associated with the buried waste. Since this heat flux is calculated using the fixed-temperature boundary condition, it is a "conservatively" high value and will result in a conservatively high temperature increase. Such an analysis indicates that the maximum temperature rise for the earth's surface will be only 0.1°F. Thus, the fixed-temperature boundary is quite satisfactory.

3.4 Input Parameters

3.4.1 Mine and Related Dimensions

In earlier studies performed by Bradshaw and Perona,¹ mine and waste container dimensions were varied over a rather wide range in an effort to establish the sensitivity of predicted temperatures to these variations. Based on those results, other related data, and more recent predictions,

Table 3.5. Description of Two-Dimensional Cylindrical Model
(Also refer to Fig. 3.3)

A. Region Definition

Region No.	Material No.	Inner R^a	Outer R^a	Upper Z^a	Lower Z^a
1	1	0	6500	0	365
2	2	0	6500	365	755
3	3	0	6500	755	1000
4b	4	0	3500	1000	1020
5	3	3500	6500	1000	1020
6	3	0	6500	1020	1070
7	2	0	6500	1070	3500

B. Description and Properties of Materials

Material No.	Description	k [Btu hr ⁻¹ ft ⁻¹ (°F) ⁻¹]	ρ (lb/ft ³)	C_p [Btu lb ⁻¹ (°F) ⁻¹]
1	Surface deposits	1.06	150	0.2
2	Shale	0.635	150	0.2
3	Salt and shale	1.85	140	0.2
4	Source	2.06	135	0.22

C. Nodal Point Locations

Node	R^a	Z^a
1	0	0
2	500	100
3	1000	200
4	1500	300
5	2000	365
6	2500	400
7	3000	500
8	3500	600
9	3750	700
10	4000	755
11	4250	800
12	4500	850
13	4750	900
14	5000	925
15	5250	950
16	5500	975
17	5750	1000
18	6000	1020
19	6250	1045
20	6500	1070
21		1100
22		1150
23		1200
24		1250
25		1300
26		1400
27		1500
28		1600
29		1800
30		2000
31		2200
32		2400
33		2600
34		2800
35		3000
36		3250
37		3500

^aDimensions are given in ft.

^bHeat generation occurs in this region.

the following sets of dimensions were selected as being suitable for a typical design analysis of the high-level mine:

Room width, ft	30	50	15
Pillar width, ft	30	50	25
Room height, ft	15	15	15
Room floor depth, ft	1000	1000	1000
Distance between floor and top of waste container, ft	8	8	8
Distance from center of container to pillar (minimum), ft	4	4	7.5
Container array	Two rows, sq. pitch	Two rows, sq. pitch	Single row
Container pitch, ft	22	42	42
Container height, ft	10	10	10
Container diameter, in.	6	6	6
Total mine area $\approx$ 900 acres			

In the actual high-level mine, dimensions of the room and pillar and the array and diameter of a given waste package will vary in accordance with the characteristics of the particular wastes that are available at any particular time. Rooms might be as wide as 50 ft and as narrow as 15 ft, while waste package diameters might range from 6 to 14 in. All such variations will eventually be considered in the thermal analysis.

The alpha waste will be stored in existing rooms that are typically 40 ft wide and 12 ft high, although room heights vary from 8 to 15 ft. The pillar widths also vary considerably but are typically 40 ft. Numerous crosscuts, about 40 ft wide, are present in the pillars. With this additional open space the average extraction ratio is about 0.75. The available gross area of the alpha facility is about 180 acres.

Various shapes and sizes of alpha waste containers are being considered. These containers will be placed, one against the other, from floor to ceiling. The remaining space in the rooms will be filled with crushed salt.

Vertical dimensioning of the general stratigraphy throughout the geologic formation is the same for the high-level mine and the alpha mine;

the data used in the calculations were based on logs from two holes at the Lyons site

3.4.2 Representation of the Stratigraphy

Some calculations have been made for the purpose of studying the effects of homogenization, shale layer insertion, etc. As shown in Fig. 3.1, discrete shale layers have been included above and below the high-level waste containers. Calculations have also been made without one or both of these shale layers. Similar calculations have been made with various discrete regions of shale and salt above the rooms. Comparisons with homogenized layers were also made in this area of the geologic formation.

3.4.3 Composition of the Region

In addition to the above variations in "region" composition, the contents of the room were varied in the 2-D model. The crushed salt was replaced with bedded salt in one case, while the entire room was filled with bedded salt in another. Also, for a 2-D (RZ) calculation, the disc shown in Fig. 3.3 was divided into 14 annular regions, each with a radial thickness of 250 ft. Starting at the center, heat sources of equal initial power density were loaded into the regions sequentially at two-year intervals. Results from this calculation were compared with those for the instantaneous loading scheme.

3.4.4 Thermal Properties

The thermal properties are discussed in detail elsewhere in this report. It suffices to say here that a few arbitrary variations in thermal conductivities, including anisotropy effects, were considered to establish the degree of sensitivity.

3.4.5 Characterization of the Waste

Both the high-level waste and the alpha waste are made up of many different radioactive nuclides; therefore, their decay curves consist of

sums of many exponential terms. At the time the high-level waste is buried, its decay rate will be somewhat greater than that for the alpha waste; consequently, temperatures associated with the former will reach a maximum at an earlier time than those for the latter.

The specific nuclide composition of the concentrated high-level waste (and hence its heat generation characteristics at the time of waste burial) will depend upon fuel enrichment, the rate and degree of fuel burnup, the length of time between reactor shutdown and reprocessing, and the time elapsed between fuel reprocessing and burial. A typical fuel for a light water reactor (e.g., the Diablo Canyon PWR) will have an initial enrichment of 3.3% ^{235}U , an average specific power of 30 MW(t)/metric ton, and a total burnup of 33,000 MWd/metric ton. It is assumed that 99.5% of the uranium and plutonium will be recovered during reprocessing and that the remainder of the actinides and fission products will be collected and solidified as high-level waste. Heat generation rates for this waste were obtained with the computer code ORIGEN,³⁹ which calculates the masses, radioactivity, and thermal power of individual fission product isotopes as a function of time, reactor type, and operating conditions. Typical output from an ORIGEN calculation is shown in ref. 40. Table 3.6 lists heat generation rates based on 12 of the specific fission products (and their daughters) and three exponentials representing the actinides; reprocessing was assumed to take place 90 days after reactor shutdown. These data were used in most of the thermal calculations. In some of the more recent calculations, all of the significant heat-generating isotopes were included and reprocessing was assumed to take place 150 days after reactor shutdown. The corresponding heat generation rates, which were used in the 50- and 15-ft-room calculations and in some of the 30-ft-room sensitivity studies, are shown in Table 3.7.

There appears to be an economic advantage in deferring burial of wastes to the maximum time permitted by federal regulations (i.e., 10 years). However, as it is possible that wastes decayed less than 10 years will be buried, such wastes must be considered in the thermal analysis.

The high-level waste can be further characterized by the chemical and physical forms of the solidified product. Oxides, glasses, powders,

Table 3.6. Transient Thermal Power of Typical Waste Resulting from the Reprocessing of Light Water Reactor Fuel

Reprocessing, 90 days after reactor shutdown

Time, t (years) ^a	$P(t)/P(t_0)$	Time, t (years) ^a	$P(t)/P(t_0)$
0	1.0	100	8.54×10^{-3}
2	0.917	110	7.19×10^{-3}
5	0.845	120	5.85×10^{-3}
7	0.800	140	4.32×10^{-3}
10	0.737	160	3.15×10^{-3}
12	0.697	180	2.52×10^{-3}
15	0.638	200	1.98×10^{-3}
20	0.576	290	5.99×10^{-3}
30	0.450	1,000	2.13×10^{-3}
40	0.351	2,000	1.07×10^{-3}
50	0.279	3,000	8.09×10^{-4}
60	0.211	4,000	7.03×10^{-4}
70	0.169	5,000	6.34×10^{-4}
80	0.132	7,500	5.03×10^{-4}
90	0.108	10,000	4.01×10^{-4}

^at is considered to be zero ten years after fuel has been discharged from reactor.

Table 3.7. Transient Thermal Power of Typical High-Level Waste from a Light Water Reactor

Reprocessing, 150 days after reactor shutdown

Time, t (years) ^a	$P(t)/P(t_0)$	Time, t (years) ^a	$P(t)/P(t_0)$
0	1.0	35	2.61×10^{-2}
0.5	0.558	40	2.31×10^{-2}
1	0.387	50	1.81×10^{-2}
2	0.225	75	9.99×10^{-3}
3	0.148	100	5.57×10^{-3}
4	0.109	200	7.91×10^{-4}
5	8.74×10^{-2}	300	2.98×10^{-4}
7	6.62×10^{-2}	400	2.16×10^{-4}
10	5.35×10^{-2}	500	1.82×10^{-4}
11	5.08×10^{-2}	600	1.59×10^{-4}
12	4.87×10^{-2}	700	1.41×10^{-4}
15	4.39×10^{-2}	800	1.26×10^{-4}
17	4.14×10^{-2}	900	1.13×10^{-4}
20	3.81×10^{-2}	1,000	1.03×10^{-4}
25	3.36×10^{-2}	10,000	2.50×10^{-5}
30	2.96×10^{-2}		

^at is assumed to be zero 150 days after fuel is discharged from reactor.

and solid products are among the variations being considered. Accompanying these variations are significant differences in thermal properties and maximum permissible temperatures.

A typical alpha waste⁴¹ will initially have the following composition: 1% ²³⁸Pu, 60% ²³⁹Pu, 24% ²⁴⁰Pu, 11% ²⁴¹Pu, and 4% ²⁴²Pu. Heat generation characteristics for such a composition are shown in Table 3.8. Data for the first 26 years (second column of table) cover the mine loading period. At the end of this period the total plutonium loading is about 38 metric tons; ref. 41 describes the loading sequence considered. The data in the fourth column in Table 3.8 give heat generation rates following mine closure, with time being measured from the date of mine closure.

The initial heat generation rate for most of the calculations was arbitrary since the temperature rises are directly proportional to power level if the thermal properties are maintained constant throughout a particular calculation. This proportionality provides a convenient means for selecting a permissible power level, consistent with temperature-change criteria, following a calculation.

4. THERMAL PROPERTIES OF THE GEOLOGIC FORMATION AND THE WASTE

The thermal properties of interest for the heat removal analysis are the thermal conductivity, k , and the diffusivity, $k/\rho \cdot C_p$, where ρ is the density and C_p is the specific heat. At present, there is some uncertainty regarding these properties for the formations surrounding the proposed Repository, particularly with respect to temperature dependence, anisotropy, and radiation damage effects. To a large extent, these uncertainties stem from the difficulties associated with making in-situ temperature-dependent determinations. Various proposals have been made for obtaining more accurate information than now exists, and experimental work is in progress. In the meantime, estimates of properties have been obtained from the literature, preliminary experiments, and data obtained from deep cores taken at the Lyons site.

Table 3.8. Heat-Generation Rate of Alpha Waste vs Time

Time (years)	Power ^a (W)	Time from mine closure = total time - 26 years	Power (W)
0	0	30	6.55×10^5
1	7.97×10^2	1×10^2	6.13×10^5
2	3.23×10^3	3×10^2	4.28×10^5
3	5.80×10^3	1×10^3	1.99×10^5
4	8.49×10^3	3×10^3	9.08×10^4
5	1.13×10^4	1×10^4	5.58×10^4
6	1.42×10^4	3×10^4	2.20×10^4
7	1.96×10^4	1×10^5	3.25×10^3
8	2.69×10^4	3×10^5	8.74×10^2
9	3.44×10^4	1×10^6	6.20×10^2
10	4.39×10^4	3×10^6	2.89×10^2
11	5.37×10^4	1×10^7	5.04×10
12	6.78×10^4	3×10^7	1.89×10
13	8.76×10^4		
14	1.14×10^5		
15	1.41×10^5		
16	1.70×10^5		
17	1.99×10^5		
18	2.29×10^5		
19	2.61×10^5		
20	2.92×10^5		
21	3.25×10^5		
22	3.59×10^5		
23	3.93×10^5		
24	4.28×10^5		
25	4.63×10^5		
26	4.76×10^5		

^aTotal power of all alpha waste considered for burial in the Repository.

In the calculations an attempt has been made to use thermal properties that would result in overestimates of the temperatures with regard to specific criteria. For instance, low thermal conductivities result in high temperatures in areas adjacent to the waste containers, and high thermal conductivities result in high temperatures at considerable distances from the mine. Because of this approach, it is appropriate to discuss the derivation of thermal properties for each mine model. A compilation of most of the properties used in the analyses of the 30-ft-room base case is presented in Tables 4.1 and 4.2. Where applicable, these data were used for both the high-level mine and the alpha mine. More recent data were used for the sensitivity studies and the 50- and 15-ft-rooms.

4.1 Three-Dimensional and Two-Dimensional (XZ) Models

The detailed nature of all of the 3-D and most of the 2-D (XZ) problems required the use of pure shale, pure salt, crushed salt, and calcine (solidified waste) properties. The general region above the room, which contains many alternate layers of salt and shale, was simulated with two homogenized regions - one containing 80% salt and 20% shale and the other containing 50% salt and 50% shale. Since most of the heat in this area moves vertically, the discrete regions were homogenized, assuming the materials to be in series. Thus,

$$k_v = \frac{k_1 k_2}{f_1 k_2 + f_2 k_1}, \quad (4.1)$$

where

k_v = thermal conductivity for homogenized region,

k_1 = thermal conductivity for salt,

k_2 = thermal conductivity for shale,

f_1 = volume fraction of salt,

f_2 = volume fraction of shale.

The specific heat and the density for these regions were estimated as follows:

$$\rho = f_1 \rho_1 + f_2 \rho_2, \quad (4.2)$$

$$C_p = f_1 C_{p1} + f_2 C_{p2}. \quad (4.3)$$

Table 4.1. Summary of Thermal Properties for the Assumed Isotropic Case

Material	Temperature (°F)	Conductivity [Btu hr ⁻¹ ft ⁻¹ (°F) ⁻¹]	Density (lb/ft ³)	Specific Heat [Btu lb ⁻¹ (°F) ⁻¹]
<u>Two-Dimensional RZ Model</u>				
Surface deposits	70	1.06	150	0.2
Shale	70	0.635	150	0.2
Shale and salt	70	1.85	140	0.2
Salt	300	2.056	135	0.22
<u>Three-Dimensional and Two-Dimensional XZ Models</u>				
Salt	390	1.81	135	0.22
Salt (80%) - shale (20%)	390	1.32	138	0.216
Salt (50%) - shale (50%)	212	1.01	142.5	0.21
Crushed salt	70	0.13	98	0.21
Calcine wastes		0.25	113	0.22
Shale		0.635	150	0.2

Table 4.2. Thermal Properties of NaCl as a Function of Temperature

Temperature (°F)	Conductivity [Btu hr ⁻¹ ft ⁻¹ (°F) ⁻¹]	Specific Heat [Btu lb ⁻¹ (°F) ⁻¹]
-58		0.198
32	3.53	
77		0.208
122	2.90	
212	2.43	
302	2.08	
392	1.80	
482	1.60	
572	1.44	
662	1.33	
752	1.20	
1472		0.260

The thermal conductivity values for pure salt were taken from ref. 42, and the density and specific heat values were taken from ref. 43. Table 4.2 shows the temperature dependence for k and C_p .

Values for the specific heat and the density of shale were taken from ref. 43. No information on temperature dependence is available. The thermal conductivity for shale was obtained using temperature profiles from two test holes at the Lyons site and an estimate of the geothermal heat flux in that area. (This is discussed in greater detail in connection with the thermal properties used for the 2-D models. It suffices to say here that no thermal dependence data are available.)

The thermal conductivity for crushed salt was estimated from an experiment conducted at ORNL.⁴⁴ The uncertainty associated with the experiment was quite large; thus the value used in the calculations is considered to be significantly less than the actual value. No data for temperature dependence were obtained.

Properties for the calcine (solidified waste) were obtained from a compilation of data by Schneider⁴⁵ for various types of solidified wastes. Temperature dependence was not considered.

Temperature dependence for the salt was considered in the 3-D and 2-D (XZ) calculations. In the region containing 50% salt and 50% shale, properties corresponding to a temperature of about 212°F were used. In the 80%-20% region and for all pure salt regions, a temperature of about 390°F was used for determination of thermal properties.

4.2 Two-Dimensional (RZ) Model

The 2-D (RZ) model generally considered the following five regions: surface deposits, shale, salt and shale, the disc source embedded in the salt-and-shale region, and another region of shale. With the exception of the source, the boundaries of the region were defined by temperature profiles obtained from two test holes at the Lyons site.⁴⁶ These profiles are shown in Fig. 4.1. It had been estimated⁴⁴ that the geothermal heat flux at the Lyons site was 1.3×10^{-2} Btu hr⁻¹ft⁻². Using this value and the temperature gradients in Fig. 4.1, the thermal conductivity for each of the indicated regions was calculated for the ambient temperature.

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Fig. 4.1. Temperatures Measured in Two Test Holes at Lyons, Kansas.

The salt-and-shale region consists of salt and shale at an estimated ratio of 2:1. Using a temperature of 70°F for the salt, the density and the specific heat were calculated for the salt-shale mixture in the same manner as described previously for the 3-D problems.

Density and specific heat values for shale were taken from ref. 43. It was assumed that the surface deposits had the same values.

The data in Fig. 4.1 indicate that the thermal conductivity of the lower shale layer is different from that for the upper shale layer. Actually, the lower portion of the curve had very few data points; thus, for the calculations, it was assumed that the properties of the material in the lower region were the same as those of the upper shale layer.

The source region was embedded in the central portion of the salt-and-shale region, and it was considered to be pure salt with properties corresponding to a temperature of 300°F.

In all of the 2-D (PZ) calculations, except those including an arbitrary change in thermal properties, ambient temperatures (those given in Fig. 4.1) were used to evaluate thermal properties for all regions but the source. This results in low temperatures at locations near the source but high temperatures at locations some distance away.

4.3 Variations in Thermal Properties

4.3.1 Recent Data from the Lyons Site

In mid-March 1971, ORNL received additional data pertaining to the two test holes at the Lyons site. The data consist of measured thermal conductivities, including information on anisotropy, for 65 zones in one hole and 25 zones in the other. A few density values are also included. The geothermal heat flux at the Lyons site was determined from this and related information to be about 2.0×10^{-2} Btu hr⁻¹ft⁻².⁴⁷ This is 50% greater than the previously estimated value of geothermal heat flux. Thus, the thermal conductivities obtained from the thermal gradients in Fig. 4.1 should be increased by about 50%. Thermal conductivities consistent with this correction are presented in Table 4.3.

Table 4.3. Summary of Thermal Properties for the
Assumed Isotropic Case -- Most Recent Values

Material	Temperature (°F)	Thermal Conductivity [Btu hr ⁻¹ ft ⁻¹ (°F) ⁻¹]
<u>Two-Dimensional (RZ) Model</u>		
Surface deposits	70	1.59
Shale	70	0.953
Shale and salt	70	2.78
Salt	300	2.06
<u>Three-Dimensional and Two-Dimensional (XZ) Models</u>		
Salt	390	1.81
Salt (80%)-shale (20%)	390	1.53
Salt (50%)-shale (50%)	212	1.37
Crushed salt	70	0.13
Calcine waste		0.25
Shale	70	0.953

4.3.2 Thermal Conductivity Anisotropy

As discussed in Sect. 4.1, regions of the geologic formation that consisted of multiple layers of salt and shale were homogenized for the 3-D model; series resistance was assumed. This yielded Eq. (4.1) for the effective thermal conductivity in the vertical direction. The same thermal conductivity was used for the horizontal direction.

In a more general case, one can consider different thermal conductivities for the vertical and horizontal directions; and, since the transients are very slow, steady-state relations for parallel and series conductivities can be used. The effective thermal conductivity in the horizontal direction for the multilayered region is:

$$k_h = f_1 k_1 + f_2 k_2 . \quad (4.4)$$

Because the shale itself tends to be a layered material, it also exhibits anisotropic properties. At about 74°F, the ratio of horizontal to vertical thermal conductivity is approximately 1.5.⁴⁸ For higher temperatures, the ratio is less,⁴⁹ but there is essentially no detailed information available. The value of 1.5 was used for the purpose of determining the sensitivity of calculated temperatures to anisotropy. Thus, Eq. (4.4) becomes:

$$k_h = f_1 k_1 + 1.5 f_2 k_2 , \quad (4.5)$$

where k_2 is the thermal conductivity of shale for the vertical direction.

By using the information at hand (Table 4.4) and considering the updated properties associated with Fig. 4.1, a new set of thermal conductivities was calculated for the three basic calculational models.

4.3.3 Changes in the Crushed Salt

Crushed salt has been proposed as a backfill material both in the rooms and around the high-level waste packages. As the result of increasing temperatures and pressures and the presence of moisture (brine from minute brine cavities), the crushed salt will densify and eventually will recrystallize, presumably ultimately achieving bedded-salt properties.

Table 4.4. Summary of Thermal Conductivities
for the Anisotropic Case

Material	Temperature (°F)	Thermal Conductivity [Btu hr ⁻¹ ft ⁻¹ (°F) ⁻¹]	
		In the Vertical Direction	In the Horizontal Direction
<u>Two-Dimensional (RZ) Model</u>			
Surface deposits	70	1.59	1.59
Shale	70	0.953	1.43
Shale and salt	70	2.78	3.09
Salt	300	2.06	2.06
<u>Three-Dimensional and Two-Dimensional (XZ) Models</u>			
Salt	390	1.81	1.81
Salt (80%)-shale (20%)	390	1.53	1.73
Salt (50%)-shale (50%)	212	1.37	1.95
Crushed salt	70	0.13	0.13
Calcine waste		0.25	0.25
Shale	70	0.953	1.43

The time required for this change to take place is not known accurately. However, results from experiments conducted during the Salt Vault Project⁵⁰ and at Hutchinson⁵¹ indicate that the change will be completed in the backfill area around the waste packages in about 100 days. More precise data need to be obtained because the variation in temperature drop across the backfill is significant for high-level waste packages with a power of 2 kW or more.

The crushed salt that is used to backfill the rooms will presumably take much longer to recrystallize, perhaps as much as 100 years.⁵² In the calculations it was assumed that there was no change in properties prior to peaking of the temperatures in the local mine area.

4.3.4 Radiation Damage to Salt and Waste

Salt within several inches of a waste package will be exposed to radiation doses that may appreciably change the thermal properties. Essentially no data exist for radiation damage of salt; however, based on data for other materials, it is estimated that the thermal conductivity might be reduced by a factor of 2 in the absence of brine migration.⁵³ Brine cavities in the salt migrate along temperature gradients in the direction of increasing temperature by two processes, dissolution of salt at the hot end of the cavity and precipitation at the cold end. Dissolution tends to remove the effects of radiation damage; thus, with the two processes taking place simultaneously, a lower degree of radiation damage exists. It has been estimated that brine-migration annealing will be effective for at least 50 years, and the actual damage during this time will be only one-sixth to one-tenth of what it might be otherwise.⁵⁴ After 50 years, the power in the waste package will be sufficiently low that a considerable reduction in thermal conductivity will probably not be objectionable.

At the present time there is no detailed information regarding radiation damage to the solidified waste. The damage is not expected to be excessive; however, more data concerning radiation damage with regard to its effects on thermal properties must be developed for both the salt and solidified waste before waste burial design details can be completed.

5. CRITERIA RELATED TO THERMAL ANALYSIS

Criteria are required in order to facilitate interpretation of the results obtained from thermal analysis. These criteria are derived from studies that consider the effects of temperature increases on the various factors influencing the allowable heat release rate (see Sect. 1). As the calculations associated with these factors are refined, new criteria are generated for use in the thermal analysis. A set of tentative criteria is given below.

5.1 High-Level Mine

5.1.1 Waste Container Temperatures

At present, the maximum permissible temperature of the solidified waste is specified as the maximum temperature that existed during the waste solidification process. It appears that this temperature will range between 1100 and 2000°F, the specific value depending upon the nature of a particular waste.

5.1.2 Formation Temperatures

Previous thermal and rock mechanics studies indicate that the salt temperatures at a position 8 in. from the container surface and at a point midway between the containers should be no greater than 480 and 390°F, respectively, in order to (1) prevent excessive migration of brine to the containers, (2) ensure stability of the mine during operations, and (3) avoid undesirably high temperatures in adjoining formations and overlying freshwater aquifers.

5.2 Alpha Mine

Alpha wastes will initially consist solely of noncombustible materials that are chemically and thermally stable to at least 390°F. Experimental investigations completed to date indicate that, in the future, it may be possible to accept certain types of combustible wastes as well, provided

they are packaged in proper containers and their temperatures are not allowed to exceed 350°F.^{55,56}

The limitations on salt temperatures for the alpha mine are the same as those for the high-level mine.

6. TYPICAL RESULTS OBTAINED FROM THERMAL ANALYSIS

Eventually the thermal analysis must consider all reasonable types of waste with regard to type of material, waste container size, initial power level, age, etc. The intent will be to minimize the total cost of solidifying, packaging, shipping, and burial, while achieving the required degree of safety. Thus far, calculations have been made primarily for the purpose of demonstrating feasibility and examining the sensitivity of the results to variations in the calculational models, stratigraphy, thermal properties, and solidified waste characteristics. The results indicate that, some distance from the local burial area, the temperatures in the geologic formations are essentially independent of room, pillar, and waste detail, and even reasonable variations in thermal properties and stratigraphy provided the temperature criteria in the burial area are met. The important independent variable is the average initial power density in the mine, and hence the initial total power, when a specific repository size is considered. With regard to temperatures in and near the waste containers, there is a greater dependence on local detail. However, it appears that the criteria can always be satisfied by varying room, pillar, and waste container dimensions, waste burial arrays, and initial power per container. Therefore, for the purpose of demonstrating feasibility, it is sufficient here to report detailed results for only a few typical cases for the high-level mine and the alpha mine and to discuss generally some of the more important perturbations. Most of the high-level mine calculations discussed in this report were made for the 30-ft-wide room. A typical set of dimensions, properties, etc., which constituted a base case, was established. The sensitivity studies were conducted using the 30-ft room. Fifty- and fifteen-foot rooms were also considered, but more from the standpoint of a variation in dimensions than as a detailed study of different room sizes.

In the following discussion of temperature variations, reference is made to temperature changes relative to the original ambient values. The changes are nearly proportional to power level, thus permitting a convenient means for scaling. Temperatures per se can be obtained using the initial ambient temperatures (given in Fig. 6.1) for the geologic formation. It is observed that, at the mine level, the initial ambient temperature is about 74°F. Thus, with reference to Sect. 5, it is seen that the maximum permissible temperature rise in the high-level waste package is about 1000 to 2000°F, depending upon the waste solidification process; it is 410°F in the salt at a point 8 in. from the surface of the waste container, and 320°F midway between the containers. The maximum permissible temperature rise in a package of combustible alpha waste is about 275°F.

Temperatures in the waste package at the time of burial will actually be significantly higher than the ambient temperature of the mine. Upon insertion of the package and backfilling of the annular void with crushed salt, the temperature of the package will decrease very quickly to the values given in this report.

In the presentation of the calculated temperatures, reference is made to specific positions on the X,Y,Z and R,Z coordinate axes. The reader is referred to Figs. 3.1-3.5 for proper spatial orientation.

6.1 Results for a 30-ft-wide Room in the High-Level Mine - The Base Case

A typical case for the high-level mine considered burial of 10-year-old Diablo Canyon waste in a 30-ft-wide room. This case, referred to as the base case, is further characterized by the dimensions and stratigraphy indicated in Figs. 3.1 and 3.3 and by the heat generation curve and thermal properties given in Tables 3.1 and 3.6. In addition, the waste container diameter was 6 in., and the solidified waste was a type of calcine, which tends to have relatively low thermal conductivity and a relatively low maximum permissible temperature (1100°F). The corresponding three-dimensional model stratigraphic and backfill characteristics were selected so as to result in conservatively high temperatures in the local salt

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Fig. 6.1. Geologic Formation Temperatures Prior to Burial of Waste.

formation, but it was assumed that rock salt was in contact with the waste container from the outset (a somewhat optimistic assumption). Thermal properties used in the 2-D (RZ) calculation were selected to give conservatively high temperatures at the earth's surface and in the aquifers. Furthermore, it was assumed that all of the waste in the mine was identical and that it was all loaded at the same time. The temperature dependence of the thermal properties and the effects of anisotropy and radiation damage were neglected for the base case but have subsequently been considered.

The thermal analysis establishes a maximum permissible initial power level per waste package for a particular set of dimensions and criteria. The base case considered here can, according to the calculations, accommodate 2000 W per waste package and thus about 130 kW per acre. It is desired, although not necessary, to bury the equivalent of about 100 MW of 10-year-old waste in the Repository. Thus, about 800 acres would be required. (If the waste has decayed less than 10 years at the time of burial, more acreage will be required for the same volume.)

6.1.1 Temperatures in the Vicinity of the Mined Area

Temperatures in the vicinity of the mined area were obtained as a function of time, primarily with the 3-D calculational model shown in Fig. 3.1. Results from the 3-D calculations for the typical case are presented in Figs. 6.2-6.5.

Figure 6.2 shows temperature changes with time at points in and near the waste containers at a mine level corresponding to the horizontal mid-plane of the waste container ($Z = 1013$ ft). It is observed that the temperature of the center of the waste reaches a maximum in about 12 years, attaining a rise of 540°F as compared with a minimum limiting value of 1000°F . At 8 in. from the edge of the container, the temperature reaches a maximum in 30 years, and the corresponding temperature increase is 365°F as compared with a limiting value of 410°F . Midway between the containers ($X = 0, Y = 0$), the temperature reaches a maximum at 40 years with a temperature rise of 328°F . This slightly exceeds the permissible value of 320°F . The shaded area in Fig. 6.2 indicates the degree of symmetry

Fig. 6.2. Temperature Rise vs Time for a 2000-W Waste Package at $Z = 1013$ ft and $X = 0$ to 30 ft.

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Fig. 6.3. Radial Temperature-Rise Profiles in the Vicinity of a 2000-W Waste Package for Time = 30 Years and Z = 1013 ft.

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Fig. 6.4. Selected Temperature Profiles for a 2000-W Waste Package in Vertical Planes Parallel to Length of Room (YZ Plane) for Time = 50 Years.

Fig. 6.5. Isotherms in the XZ Plane at $Y = 0$. Time after burial, 50 years; base case, 2000 W.

around the container in the XY plane. At a radial distance of about 11 ft from the container, the maximum variation in the temperature is only 20°F. This symmetry is also observed in Fig. 6.3, which shows radial temperature profiles around the container at 30 years and out to a distance of about 5 ft.

Figure 6.4 shows temperature profiles in the Y direction at 50 years for different values of X and Z. It is evident from this figure that temperature gradients in the Y direction are essentially zero for areas a few feet (~5 ft) away from the source.

Figure 6.5 depicts the mine in the XZ plane at $Y = 0$ and shows isotherms at 50 years. As indicated, the temperature gradients in the X direction within the pillar are nearly zero. From this information and that in Fig. 6.4, the average temperature increase in the pillar at 50 years is determined to be about 285°F. This is the peak value achieved.

Results from a 2-D (XZ) calculation that used the same regions, materials, and mesh spacings but represented the waste package with a vertical slab (as described in Sect. 3) are essentially the same as those above, up to a few feet from the container. A comparison of the temperature increases at a few specific points is presented in Table 6.1. If the temperatures for the 3-D model are averaged in the Y direction with the weighting indicated in Fig. 6.3, the temperatures near the container are in good agreement. Thus the 2-D (XZ) model can be very useful for parametric studies in the mine area.

6.1.2 Temperatures Outside the Immediate Mine Area

Temperatures obtained with the 2-D (RZ) model for the area surrounding the mine are shown in Figs. 6.6-6.8. Each of these figures represents vertical temperature-rise profiles extending from the surface of the earth to several hundred feet below the waste container. Results of the analysis indicate that, several years after the entire disposal area is full, the radial temperature distributions above and below the mine area will be essentially flat to within about 500 ft of the edge of the mine. Figure 6.6 shows the vertical temperature profiles for this area; as indicated

Table 6.1. Comparison of 3-D(XYZ) and 2-D(XZ) 30-year
Temperature Rises for 2000 W per Can

Location	Temperature Increase (°F)		
	3-D		2-D
	Y = 0 ft	Y = 11 ft	
A	324.6	321.6	322.8
B	402.4	320.6	335.4
C	363.4	318.2	327.2
D	359.0	318.2	327.0
E	329.0	316.2	321.2
F	304.0	303.8	303.6
G	247.8	247.8	247.6
H	176.6	176.6	176.4

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Fig. 6.6. Temperature-Rise Vertical Profiles for 2000-W Waste Packages at Center of Disposal Area.

Fig. 6.7. Temperature-Rise Vertical Profiles for 2000-W Waste Packages 500 ft Beyond Edge of Mine.

Fig. 6.8. Temperature-Rise Vertical Profiles for 2000-W Waste Packages 1750 ft Beyond Edge of Mine.

in this figure, the peak temperature increases in the region containing freshwater aquifers (down to 500 ft below the surface) are in the range $< 30^{\circ}\text{F}$, assuming that the aquifers are stagnant. Because the heat flux in this region is very low, only a small aquifer flow rate would be required to essentially eliminate the temperature rise in this region. It is also observed that a period of 100 years would be required for a perceptible increase in the temperature of a stagnant aquifer to take place, whereas 700 years would be required to reach the peak.

Figure 6.7 shows the vertical temperature profiles 500 ft from the edge of the mine. The shortest time to attain the peak temperature is about 700 years, and the corresponding temperature rise is about 20°F . At 1750 ft from the edge of the mine (Fig. 6.8), the minimum peak time is about 3000 years and the corresponding temperature increase is 2.5°F .

In Fig. 6.6 it is observed that the surface heat flux peaks in about 700 years. Its value is estimated from the slope of the temperature curve to be $0.22 \text{ Btu hr}^{-1}\text{ft}^{-2}$. As indicated in Fig. 6.9, the surface heat flux resulting from waste burial is essentially zero for the first 100 years. After the peak value occurs, the heat flux decreases very slowly, with 1300 years being required for reduction by a factor of 2. Figure 6.10 shows how the peak surface heat flux varies with horizontal distance from the center of the mine; at a short distance (500 ft) beyond the edge of the mine, the peak value is lower by a factor of 5.

The rise in surface temperature associated with the added surface heat flux has been calculated to be about 0.2°F . It is of interest to note that the peak heat flux at the surface is about 12 times the geothermal heat flux ($2.0 \times 10^{-2} \text{ Btu hr}^{-1}\text{ft}^{-2}$) and about 500 times less than the solar heat flux.

Fig. 6.9. Relative Surface Heat Flux Above the Center of the High-Level Mine.

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Fig. 6.10. Peak Surface Heat Flux as a Function of Horizontal Distance from the Center of the Mine.

6.2 Results of the Sensitivity Study for the High-Level Mine

Sensitivity studies have been conducted for the purpose of considering perturbations and variations in the following parameters: (1) shale layer thickness above and below the waste package (see Fig. 3.1), (2) room content (crushed salt and void, bedded salt and void, or all bedded salt), (3) backfill around waste container, (4) mine loading sequence, (5) thermal conductivity (temperature, anisotropy, radiation damage, and general uncertainty effects), (6) transient thermal power of the waste, (7) age of waste at burial, and (8) room and pillar dimensions. Items (7) and (8) are somewhat out of the realm of sensitivity studies and thus are discussed in separate sections.

6.2.1 Variations in Thickness of the Shale Layer in the Vicinity of the Waste Package

Shale layers close to the waste package tend to insulate the enclosed region since the thermal conductivity of shale is lower than that for salt. The layer thicknesses assumed for the base case are considered to be overestimates. Calculations indicate that removal of one or both of the layers has little effect on the temperatures, the maximum temperature change in the salt being only 9°F (2%). Temperature differences at various positions are shown in Table 6.2.

Variations in room content have a somewhat greater effect. The most severe condition expected with regard to temperatures near the waste package is that used for the base case. With time the void will be replaced with salt, and the crushed salt will recrystallize, improving the thermal conductivity substantially. As shown in Table 6.3, if this latter condition existed from the outset, the peak temperature at the container surface would be about 30°F (8%) lower; and, at the point of maximum positive difference, which is located a few feet above the pillar, the peak temperature would be about 14°F (6%) higher as compared with the base case.

Table 6.2. Comparison of Cases at 30 Years, With and Without Layers of Shale,
Located Near Waste Container

[2-D (XZ), 2000-W waste package]

Location	Temperature Differences ^a (°F)		
	Lower Layer Removed	Upper Layer Removed	Both Layers Removed
A	-4.6	-3.8	-8.4
B	-4.4	-3.8	-8.0
C	-4.2	-4.0	-8.2
D	-5.0	-3.8	-9.2
E	-4.0	-3.8	-7.6
F	-2.8	-3.2	-6.0
G	-3.4	+3.2	-0.2
H	-4.0	+2.6	-0.4

^aTemperature for indicated case, minus temperature
with both shale layers present.

Table 6.3. Comparison of Cases, at 30 Years, for Various Room Contents

[2-D (XZ), 2000-W waste package]

Location	Temperature Differences (°F)	
	Void and Salt	All Salt
A	-12.4	-29.4
B	-10.6	-26.8
C	-11.4	-28.0
D	-10.2	-26.2
E	-9.6	-25.2
F	-7.2	-21.8
G	+4.4	+3.0
H	+5.0	+13.6

^aTemperature for indicated case, minus temperature with void and crushed salt.

6.2.2 Backfill Around the Waste Package

When a given waste package is placed in the salt the annular clearance that will exist around the container must be backfilled with some reasonably good thermal conductor. If crushed salt (which has been proposed for this purpose) is used, the thickness of the annulus might be about 2 in. The thermal conductivity of typical crushed salt is much less than that of bedded salt. If the lower value persisted, the peak temperature rise in the waste would be about 870°F and would occur at about 5 years. This condition, although more severe, appears to be acceptable. Based on experiments in the Lyons⁵⁰ and Hutchinson⁵¹ salt mines, it is expected that the crushed salt will revert to nearly bedded salt within a few months as a result of the effects of moisture, temperature, and pressure. Under these conditions, the temperature of the waste would reach a maximum even sooner, although at a value less than 870°F.

6.2.3 Mine Loading Sequence

A mine loading sequence was simulated in a 2-D (RZ) calculation by adding, at two-year intervals for 26 years, concentric equal-radial-width annuli to make up the disc source shown in Fig. 3.3. This accelerated-loading-rate scheme resulted in very little difference in temperatures as compared with those obtained with the instantaneous loading scheme used in the base case. Although additional loading sequence studies must be performed, it appears that the anticipated sequences will not have a significant effect on peak temperatures.

6.2.4 Uncertainty in Thermal Conductivity

The thermal conductivities used in the 2-D (RZ) base-case calculations and the thermal conductivity for shale used in the 3-D base-case calculations should be increased by about 50% to achieve consistency with the new estimate of the geothermal heat flux at the Lyons site. This was done in one 2-D (RZ) and one 3-D calculation. For the two-dimensional case, peak temperatures adjacent to and near the center of the disc source were 42°F (16%) less but occurred at about the same time. The peak heat flux at the earth's surface and the peak temperatures in the aquifers occurred at about

500 years instead of 700 years; and at 1750 ft from the edge of the Repository, the peak temperature occurred at 2000 instead of 3000 years. The differences in these peak values for the two cases were negligible. For the 3-D case, the peak temperature at the container surface was 27°F (7%) less, although it occurred at about the same time.

6.2.5 Dependence of Thermal Conductivity on Region

In another 3-D calculation for a 30-ft-room, an additional "region" of salt extending about 5 ft to either side of the container and to the upper and lower adjacent shale layers (similar to that shown in Fig. 3.4 for the 50-ft room), was added around the waste container. The thermal conductivity of the salt in this region was reduced to a value consistent with a temperature of 482°F. In previous calculations the thermal properties in this area were evaluated at 392°F. This change resulted in an increase in the container peak surface temperature of 12°F (3%); however, the time at which the peak occurred remained essentially the same.

6.2.6 Thermal Conductivity Anisotropy

Thermal conductivity anisotropy in shale was included in a 2-D (RZ) and in a 2-D (XZ) calculation, assuming that the ratio of horizontal to vertical thermal conductivities was 1.5. The regions in the models that exhibit anisotropic properties and the thermal conductivities used are shown in Figs. 3.3 and 3.2 and Table 4.4. The results of the calculations indicate a peak temperature rise of 3.3°F at a position 1750 ft from the edge of the mine as compared with 2.5°F at the same position when anisotropic effects are disregarded. Temperatures close to the source and near the center of the mine, all the way to the earth's surface, were essentially the same. Thus, it appears that the effects of anisotropy are negligible within the range considered.

6.2.7 Effects of Radiation Damage on Thermal Conductivity

The gamma radiation of salt will presumably cause radiation damage, and thus a reduction in thermal conductivity, perhaps by a significant amount. However, at present, it is believed that brine migration through

the irradiated salt will reduce the radiation damage by a large factor. Preliminary estimates indicate that the net change in thermal conductivity will not present an overriding problem.

6.2.8 Dependence of Thermal Conductivity on Temperature

As discussed in Sect. 4., the thermal conductivities for the various salt regions were held constant during the transient calculations. The particular values that were selected were not necessarily temperature- and time-averaged. Rather, they were the values that presumably would result in conservatively high temperatures at particular points of interest. Certainly more representative values could have been selected if the calculation of nominal temperatures had been the goal, and the accuracy could have been increased by adding more material regions (see Sect. 6.2.5). The "extreme" in this direction is to allow the thermal conductivity to change with temperature at every nodal point and time step. Such a procedure is to be avoided as much as possible because of the large amount of additional computer time required. However, a few cases were calculated in this way to provide a check on the degree of conservatism and to help select appropriate average values for future calculations.

Results from 2-D (XZ) calculations show that the detailed temperature dependence reduced the peak temperature at the surface of the waste container by 13°F (3%), as compared with results for the base case. The peaks still occurred at about the same time. Midway between the waste containers ($X = 0$, $Y = 0$), the difference was 12°F. The biggest difference occurred earlier in the transient, when the temperatures are lower and the difference in thermal conductivities is larger. A maximum difference of 25°F (9%) was achieved at the surface of the waste container in about 5 years.

Results from 2-D (RZ) calculations show that including the effects of temperature makes essentially no difference in temperatures near the earth's surface, in the aquifers, and at a position 1750 ft beyond the edge of the mine. The times at which the temperature peak are also essentially the same.

6.2.9 Stratigraphy Representation

Results from 2-D (RZ) calculations were used to study the effects of homogenization above the mine area. Three cases were calculated in which the geologic formation between $Z = 400$ and $Z = 1000$ ft was assumed to be 50% salt and 50% shale. For one of these cases, the 600-ft region was divided into 20-ft-thick alternate layers of salt and shale. In the second case, the region was homogenized using series resistance; and for the third case, the upper 300 ft was shale and the lower 300 ft was salt. The results show that the maximum percentage differences in temperatures occur near the source at the time the source temperatures peak (~50 years). The difference relative to the multilayer case was +5% for the homogenized case and -20% for the two-region case. This type of information provides a guide to proper modeling of the stratigraphy.

6.2.10 Characteristics of Heat Generation Decay

The values for heat generation decay considered in most of the calculations thus far are those given in Table 3.6. The more recent estimates presented in Table 3.7 were used in similar problems to evaluate the associated differences in results from the thermal calculations. A comparison of the heat generation values in the two tables indicates a more rapid decay for the more recent heat generation curve. This means that use of the latter curve will result in peak temperatures that occur somewhat sooner and that, for the same initial power per container, the total energy (and hence temperatures) will be less. Results from the 3-D calculations for a power of 2000 W show that the peak temperature at the container surface is 11°F (3%) less and occurs about 7 years sooner. The temperature differences at positions farther away from the heat source are less, and the peaks occur more nearly at the same time.

6.3 Two-Dimensional (XZ) Analysis of the High-Level Mine for a 1-year-old Waste

It is possible that high-level waste aged less than 10 years will be buried in the Repository. As indicated in Table 3.7, this waste will have a shorter effective half-life, which will cause temperatures to reach a maximum sooner but at a lower value for a given initial power level. Of course, a given quantity of reprocessed fission products will have a higher specific power at shorter decay times. Thus, from an economic point of view, it would be desirable to use a higher initial power for waste aged less than 10 years.

A 30-ft-room case was calculated using a 1-year-old Diablo Canyon waste. Results from the 2-D (XZ) model (see Fig. 3.2) indicate that the temperature at the surface of the container reaches a maximum in about 1 year as compared with 25 years for the 10-year-old waste. At a location midway between the waste packages, the peak occurs at about 2 years as compared with 40 years. Based on the same temperature criteria considered for the above base case with 10-year-old waste, the permissible initial power level was about 4000 W; the limiting point is a point 8 in. from the container surface. The peak waste temperature limited the power to 5000 W, and the peak temperature midway between containers limited the power to 9000 W. Increasing the container diameter decreases the temperature at the 8-in. point relative to the temperatures midway between the containers. Thus, by increasing the diameter of the waste container, the permissible power level might be increased to 5000 W per waste package.

Table 3.7 shows that the specific power of a 10-year-old waste is about a factor of 7 less than that for 1-year-old waste. However, as indicated above, the initial permissible specific power for 1-year-old waste is only about 2.5 times that for the older waste. Therefore, according to these calculations, about three times as much 10-year-old reprocessed fission product waste can be buried in a given volume of mine space as waste aged only 1 year. It is possible, though, that burial optimization will result in a somewhat different ratio.

Peak temperatures outside the immediate mine area are the same for the 5000-W, 1-year-old waste case as they are for the 2000-W, 10-year-old waste case. However, the peaks occur somewhat sooner for the 1-year-old waste.

6.4 Three-Dimensional Analysis of the High-Level Mine for a 50-ft-wide Room

Three-dimensional calculations were made for a 50-ft-wide room with two rows of waste packages arranged on a square pitch of 42 ft. The pillar width was also 50 ft, and 10-year-old waste in a 10-ft-long by 6-in.-diam container was considered. The detail of the model is shown in Fig. 3.4. A comparison of Fig. 3.4 with Fig. 3.1 shows that an additional region, which surrounds the waste package, was added to the 50-ft-room model. This region was added to facilitate a better representation of the thermal conductivity of salt at the level of the source, where temperature gradients are largest.

The thermal conductivity for shale was based on the temperature gradient data in Fig. 4.1, using the most recent prediction for the geothermal heat flux (2.0×10^{-2} Btu hr⁻¹ft⁻²). A summary of the thermal properties used in the 50-ft-room analysis is presented in Table 4.3.

Results from the 3-D analysis are shown in Fig. 6.11 for a power of 5000 W per waste package. It is observed that, at a position 8 in. from the waste container surface, the peak temperature rise occurs in 10 years and is 410°F, precisely the maximum permissible value. Midway between the waste packages (at $X = 0$, $Y = 0$), the peak temperature rise occurs at 35 years and is only 235°F, well below the permissible value of 320°F. The peak temperature rise at the center of the waste is 1100°F, and it occurs in less than one year, assuming that bedded salt is placed adjacent to the container and that radiation has caused no damage (i.e., no reduction in thermal conductivity) to the salt. This temperature rise is somewhat in excess of the permissible value (i.e., 1000°F), indicating that a solidified waste having a higher thermal conductivity and/or a higher permissible temperature should be used. At the time that the

Fig. 6.11. Temperature Rise vs Time for a 5000-W Waste Package at $Z = 1013$ ft. Room width, 50 ft; spacing, 42 ft.

temperature reaches a maximum in the waste, the temperature drop through the waste for the calculated case is about 530°F.

Assuming that solidified waste having a higher thermal conductivity is used, the particular arrangement with 5000 W per waste package satisfies the tentative criteria and yields an acceptable initial power per acre (104 kW/acre), which is less than that for the case of 2000-W packages in 30-ft rooms. The value for the 5000-W case can probably be increased by increasing the diameter of the container; this will reduce the temperature at the position 8 in. from the container surface and thus permit a smaller room and pillar size and a smaller pitch for the waste package.

Since the power per acre for the calculated case is less than that for 2000-W packages in 30-ft rooms, the temperatures in the geologic formation at locations some distance from the immediate mine area will be less than those calculated for the latter case.

6.5 Three-Dimensional Analysis of the High-Level Mine for a 15-ft-wide Room

Results from the preceding 50-ft-room case indicate that, for high-power packages, more power per unit area of mine could be achieved by using a single row of packages in a very narrow room. The minimum width for a room, based on equipment maneuverability, is presently specified as 15 ft, and the corresponding minimum pillar width is 25 ft.⁵⁷ A 3-D model for this combination is shown in Fig. 3.5.

The 15-ft-room case was calculated by using the above 3-D model and by assuming the same properties of materials as used for the 50-ft-room case. The waste packages were placed in a single row at the middle of the room with a distance of 42 ft between them. This spacing is the same as that used for the 50-ft-room case. The results from the calculations are shown in Fig. 6.12 for a power level of 5000 W. As indicated, the peak temperatures in and adjacent to the waste package are slightly less than those for the 50-ft-room case, while those farther away are somewhat greater. At the center of the waste package and at a position 8 in. from the

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Fig. 6.12. Temperature Rise vs Time at $Z = 1013$ ft. Power, 5000 W; room width, 15 ft; spacing, 42 ft.

container surface, the peak temperature rises are about 5% higher than the permissible values of 1000°F and 410°F respectively. Midway between the package, the peak temperatures are well below permissible values. Thus, if no other changes are made, the power per package should be reduced from 5000 W to 4800 W. Based on this power level, the permissible initial loading for an infinite array of 15-ft rooms is 124 kW/acre, which is nearly the same as that for 2000-W packages in a 30-ft room. However, this value is 20% greater than that obtained for 5000 W in a 50-ft room. Furthermore, 40% less salt needs to be mined (exclusive of corridors) per waste package in a 15-ft room as compared with that for a 50-ft room. Thus, the 15-ft room appears to be more economical for ~5000-W waste packages.

6.6 Results for the Alpha Mine

A one-dimensional model similar to the 2-D (RZ) model was used to calculate temperature rises for the alpha mine. The detail of the model in the vertical direction was essentially the same as that shown in Fig. 3.3. The source was loaded instantaneously with a total power of 0.476 MW, which is the power level at the time of mine closure (see Table 3.8). The power density was based on a gross mine area of 180 acres. Results from the calculations indicate that peak temperature rises at the center of the mined area and at a point 300 ft below the earth's surface will occur at about 1000 and 1500 years, respectively. The corresponding temperature rises are 37°F and 9°F.

The average power density in the alpha waste before compaction is estimated on the basis of information in ref. 41 and Table 3.8 to be 0.0042 W/ft³. In ref. 41, it is proposed that much of the waste be compacted by a factor of 10. Assuming a thermal conductivity of only 0.1 Btu hr⁻¹ft⁻¹(°F)⁻¹ for the compacted material and a minimum dimension of 10 ft for the waste package conglomerates in the room, the maximum temperature decrease in the waste is nominally only 20°F. Therefore, the nominal peak alpha waste temperature will be well below the permissible value of 350°F. Furthermore, the peak surface heat flux and temperature rises in the aquifers and in areas outside the Repository are considerably below those calculated for the high-level mine.

6.7 Accuracy of Numerical Solutions

The three finite difference techniques used thus far for solving the heat conduction equation (see Sect. 2.) satisfy the basic requirement of convergence. That is, each converges to the true solution of the differential equation as the spatial increments and the time increments approach zero. The remaining question is how small these increments must be to achieve a certain degree of accuracy. Unfortunately, there is not a simple answer to this question; however, various methods are available for estimating the accuracy and for developing confidence in the technique. Some of these methods, as applied to the heat conduction problem in the Repository, are discussed below. It is tentatively concluded, based on such analyses in connection with the problem at hand, that the error will be less than 2% if doubling the space increments or decreasing the time increments by a factor of 2 results in temperature changes less than or equal to 2%. This is the convergence criterion that is presently used.

6.7.1 Comparison of Numerical and Analytical Solutions

Comparisons of numerical and analytical solutions can be accomplished only for relatively simple models. However, such comparisons are useful, and several have been made for the Repository. In a typical case, the Repository consisted of an infinite homogeneous slab source at a depth of 1010 ft in a semi-infinite medium of shale, and the heat generation decay was represented by two exponential terms. The analytical transient solution was obtained⁵⁸ using Green's functions, and the same problem was solved numerically with the HEATING code.⁶ A comparison of calculated temperatures obtained for the two methods is shown in Table 6.4 for depths of 510 and 1010 ft below the earth's surface and for times after burial up to 2000 years. As indicated in the table, two sets of space-time increments were used in separate numerical solutions. For temperature rises greater than 1°F, the agreement between the three sets of numbers is better than 1%.

It should be pointed out that the "analytical" solution referred to is not truly analytical in that an infinite series must be evaluated. However, a sufficient number of terms was used to achieve the number of significant figures shown in the table.

Table 6.4. Comparison of Temperature Rises Calculated with a Finite Difference Technique and an Analytical Technique

Time (years)	Temperature Rise (°F)					
	Distance Below Surface of Earth					
	510 ft			1010 ft		
	Finite Difference Technique			Finite Difference Technique		
	59 Nodes, $\Delta t = 1$ year	100 Nodes, $\Delta t = 0.1$ year	Analytical Method	59 Nodes, $\Delta t = 1$ year	100 Nodes, $\Delta t = 0.1$ year	Analytical Method
30	0.0005	0.0002	0.000302	392.75	393.50	390.5
34	0.0019	0.0010	0.00134	394.97	394.94	392.0
50	0.0580	0.0480	0.0514	384.24	382.47	379.6
150	11.64	11.60	11.52	235.28	233.42	231.5
300	38.84	38.71	38.34	152.06	151.02	149.9
700	55.18	54.89	54.44	99.69	99.13	98.45
2000	39.11	38.96	38.74	62.52	62.40	62.08

6.7.2 Exponential Convergence Hypothesis

Somewhat arbitrarily it was assumed that, as the time increment was decreased for subsequent calculations, the temperatures would converge exponentially to the true values. Under these conditions, an asymptote (the "true" value) can be calculated using temperatures from three different cases (different time increments). The difference between the asymptote and the calculated temperature for a particular case is the estimated error, which is obtained from:

$$\epsilon(N,t) = \tilde{\Delta T}(N,t) - \Delta T(t) = ae^{-bN}, \quad (6.1)$$

where

$N = t/\Delta t$ = number of time increments,

$\tilde{\Delta T}(N,t)$ = calculated temperature rise using N time steps to reach time t ,

$\Delta T(t)$ = asymptote corresponding to time t ,

a, b = constants.

The simultaneous solution of three such equations, each corresponding to a different value of N , yields:

$$\ln \left(\frac{\tilde{\Delta T}_{j+1} - \Delta T}{\tilde{\Delta T}_j - \Delta T} \right) = \left(\frac{N_{j+1} - N_j}{N_{j+2} - N_j} \right) \ln \left(\frac{\tilde{\Delta T}_{j+2} - \Delta T}{\tilde{\Delta T}_j - \Delta T} \right), \quad (6.2)$$

from which ΔT can be determined.

This method for estimating the error was applied to the 3-D base case for a 30-ft room, using four different values of N for $t = 50$ years. The greatest change in temperature from case to case occurred on the surface of the waste container at $Z = 1013$ ft. Two asymptotes, one using cases 1, 2, and 3 and the other using cases 2, 3, and 4, were calculated for this point. The results are shown in Table 6.5. As indicated, the difference between the two asymptotes is only 0.1%, implying that the convergence is very nearly exponential. An estimated error of 1%, which is consistent with the present convergence criteria, is achieved with $N = 480$ (case 3). This number of time steps for $t = 50$ years is also reasonable with regard to computer time.

Table 6.5. Estimated Errors Based on the
Exponential Convergence Hypothesis

Case	N	$\tilde{\Delta T}$ (°F)	ΔT (°F)	ϵ (%)
1	120	413.18	368.0 367.6	12
2	240	389.69		6
3	480	372.94		1
4	960	367.95		-0.1

6.7.3 Comparison of Results Obtained with Different Numerical Solutions

A comparison of results obtained with different finite difference techniques is also useful in developing confidence in the method of solution. The three techniques presently being used - CEP, Levy's modified CEP, and ADI - have been applied to the same problems with essentially identical results, considering the different sensitivities to mesh spacing and time increments.

In this same regard, it can be very useful to have independent analyses performed. Such an effort is under way and will be expanded considerably in the near future. It is expected that much of the independent work will be done outside of ORNL, in which case independent approaches to modeling will probably be introduced.

7. FUTURE STUDIES

The various studies conducted thus far in connection with the Waste Repository indicate that the concept is technically feasible with regard to containment capability. Future studies will be aimed at increasing the detail and improving the accuracy of the models and methods of analysis so that waste storage economics can be optimized while maintaining the required high level of confidence in the containment. Containment integrity analyses will be continued for quite some time after operation of the mine commences. These studies will make use of experimental data obtained from the site to determine whether the actual temperatures, displacements, etc., are in satisfactory agreement with predicted values.

The overall thermal analysis program for the next several years can be divided into the following general categories: (1) improvements in the modeling of the Repository, (2) improvements in the numerical solution, (3) development of more precise criteria, (4) sensitivity studies, (5) parametric studies, and (6) development of a mine-management computer program.

7.1 Improvements in Modeling

Three-dimensional models need to be developed for the proposed mine loading sequence. It appears that temperature distributions for the geologic formation during the 25-year burial period, as well as thereafter, will be important in the rock mechanics analysis. This information is also important in terms of determining the workability of the mine during the burial period. The mining and burial patterns must be such that excessive salt and atmosphere temperatures are not encountered. Improvements in all models will be made through the application of more precise stratigraphic and thermal property data as they become available. Radiation damage effects and densification and recrystallization rates for the crushed salt (backfill material) are of particular interest at this time.

7.2 Numerical Solution Techniques

The models discussed above will be considerably larger than previous models in terms of computer capacity and time requirements. Furthermore, the number of calculations required for the proposed parametric analysis is quite large. This provides economic incentive for developing and adopting faster numerical analysis techniques. As indicated in Sect. 2., the ADI technique is presently under development, and improvements in its application to the Repository problem are anticipated.

7.3 Criteria

Development of more precise criteria is becoming more important as the time approaches for making a large number of consistent calculations for an updated cost analysis for the waste disposal concept. Specific salt temperatures, as presently used, will probably be replaced with integrated volumetric expansions, volume-averaged temperatures, and specific brine migration limitations.

7.4 Sensitivity Studies

Sensitivity studies are conducted for the purpose of determining the economic incentives for improving the accuracy of the calculational model, the numerical methods of analysis, materials property data, stratigraphy detail, and the criteria. These studies are performed on a continuing basis as an integral part of the overall thermal analysis program.

7.5 Parametric Studies

The parametric studies are intended to provide preliminary information with which to "minimize" waste burial costs for all varieties of wastes. Such information is needed in the near future for waste processors and for the architect-engineer responsible for the Repository. The variables in the analysis will consist of: composition, power, age, and thermal properties of the waste; container dimensions; pitch and array of the waste packages in the mine; room and pillar dimensions; and time

and location of package burial relative to previous burials in the mine. These studies are expected to extend over a 2-year period, with preliminary information being made available in the very near future.

7.6 Mine-Management Computer Program

Some time prior to actual operation of the Repository, it may be desirable to develop a mine-management computer program that can be used during operation of the Repository for determining optimum waste-package characteristics, room and pillar dimensions, and array of the waste packages in accordance with actual waste availability.

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