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NUMERICAL MODELLING OF ROCK STRESSES
WITHIN A BASALTIC NUCLEAR WASTE REPOSITORY
PHASE II - PARAMETRIC DESIGN STUDIES

July 1978

Prepared for Rockwell Hanford Operations,
A Prime Contractor to U. S. Department of Energy,
Under Contract Number EY-77-C-06-1030

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1.0 INTRODUCTION

This report is presented as a progress report of the University of Minnesota's research contract entitled "Numerical Modelling of Rock Stresses Within a Basaltic Nuclear Waste Repository." For discussion and analytical purposes, problems associated with the parameter study were broken down into three size groups. These three scales are loosely defined as canister-scale, room-scale, and regional-scale studies. Figure 1.1 shows the base cases used for the parameter study for each scale and the number of parameters varied. A number of numerical techniques were used throughout this report. These include finite element, finite difference, closed form solutions, and boundary element techniques.

As there is no preliminary repository design established at this time as a base case, the initial parameters used for comparison throughout this report had to be selected. Section 3.0 details the material properties, waste form and geometric layouts from which variations in parameters were studied. The assumed repository consists of long rooms excavated at a single level at 1000 meters below the surface. The waste canisters are placed in holes bored in the floor along the center line of the rooms. Although this is the most commonly assumed layout used in other studies in the United States and in other countries, the first repository built in the U. S. may not have this form.

<p>BASE CASE</p> <ul style="list-style-type: none"> * Thermal studies * 1D analysis * Canister 0.4 m diameter * Canister 5 m long * Basalt-canister contact <p>CHANGES IN PROPERTIES</p> <ul style="list-style-type: none"> * Basalt conductivity * Canister conductivity <p>INFLUENCE OF AIR GAP</p> <ul style="list-style-type: none"> * Crushed rock backfill * Changes in gap width <p>BOREHOLE DECREPITATION</p> <ul style="list-style-type: none"> * Conductivity function of expansion <p>BOREHOLE LINER</p> <ul style="list-style-type: none"> * 2D analysis * With steel liner, concrete plug 	<p>BASE CASE</p> <ul style="list-style-type: none"> * Rectangular openings * Pillar width 24 m * Lithostatic stress field * Thermal loading 25 w/m² * Retrievalability 5 years * Canisters in floor * Constant basalt properties * Depth 1000 m * No ventilation of rooms <p>DIFFERENT OPENING SHAPES</p> <ul style="list-style-type: none"> * Arched roof * Circular cross section <p>REDUCED PILLAR WIDTHS</p> <ul style="list-style-type: none"> * Pillar 12 m * Pillar 6 m <p>DIFFERENT STRESS FIELDS</p> <ul style="list-style-type: none"> * MOR= 0.5 VER * MOR= 1.5 VER <p>INCREASED THERMAL LOADING</p> <ul style="list-style-type: none"> * 50 w/m² <p>DIFFERENT RETRIEVABILITY PERIODS</p> <ul style="list-style-type: none"> * 25 years * 50 years <p>VARIOUS CANISTER LOCATIONS</p> <ul style="list-style-type: none"> * Inclined vertical * In sidewalls <p>CHANGES IN BASALT PROPERTIES</p> <ul style="list-style-type: none"> * Young's modulus * Poisson's ratio * Thermal expansion <p>INFLUENCE OF DEPTH</p> <ul style="list-style-type: none"> * Increased depth <p>EFFECT OF VENTILATION</p> <ul style="list-style-type: none"> * Rooms cooled 	<p>BASE CASE</p> <ul style="list-style-type: none"> * Repository 1000 m * Vantage Sandstone * Unconsolidated sediments, 0 to 250 m * 10-year-old spent fuel <p>WASTE AGE AND FORM</p> <ul style="list-style-type: none"> * 5- and 10-year-old spent fuel * HLW and PWR/BWR mix <p>REPOSITORY SHAPE</p> <ul style="list-style-type: none"> * 3D analysis * 4 variations of repository layout <p>FORCED CONVECTION</p> <ul style="list-style-type: none"> * Convection in interbeds above repository * Convection in top flow below repository * Three flow cases <p>COUPLED HEAT AND GROUNDWATER FLOW</p> <ul style="list-style-type: none"> * Vary porosity * Release time of particles-trace path <p>COUPLED HEAT, GROUNDWATER AND STRESS</p> <ul style="list-style-type: none"> * Permeability function of stress
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FIGURE 1.1

SUMMARY OF PARAMETRIC STUDY ANALYSES

As yet, no study has been undertaken to investigate plugged versus unplugged boreholes, although the influence of the borehole lining on the temperature flow to the borehole plugging was investigated. The effect of moisture was not specifically studied here, but the influence of groundwater flow on the temperature distribution around a repository was.

Additional factors included in the parametric study were:

1. Influence of borehole diameter;
2. Basalt decrepitation;
3. Pillar size;
4. Horizontal stress ratio;
5. Influence of waste form and age on regional temperature distributions;
6. Temperature distribution changes resulting from flow in the Vantage Sandstone and flow tops;
7. Effect of porosity on the transport time for groundwater flow through the repository.

2.0 SUMMARY AND CONCLUSIONS

A parametric study of the influence of material property, geometric, and waste form parameters on temperatures and stresses was performed. The results of parametric analysis (in this report) are preliminary, utilizing the best available assumptions and data; however, they are not intended to accurately reflect actual conditions that may be encountered in the environment surrounding a repository. The base case studied is for a conventional repository with a 5-year retrievability period.

2.1 Canister Scale

1. Variation in canister thermal properties produces insignificant changes in rock temperatures and stresses.

2. Basalt thermal properties. A reduction in basalt thermal conductivity gives rise to a moderate increase in canister and rock temperature.

3. Air gap. An increase in rock-filled air gap width causes increased canister temperatures and only minor changes in rock temperatures.

4. Borehole decrepitation. A coupled thermal mechanical analysis incorporating rock failure and a reduction in thermal properties showed significant canister and rock temperature changes from the base case.

5. Borehole lining. A steel borehole liner provides a vertical conducting path; however, if the liner is approximately the same length as the canister, only minor modifications in the temperature distribution results.

6. Concrete plug. Concrete has similar thermal properties as basalt; hence the concrete plug responds thermally similarly to the basalt.

2.2 Room Scale

1. Influence of thermal loading. Increases in gross thermal loading causes significant temperature and stress increases in the floor, moderate stress changes along room walls and roof.

2. Changes in depth result in a linear increase in stresses around the room.

3. Basalt properties. Variations in the elastic rock modulus or thermal expansion coefficient produce proportional changes in the thermally induced stresses. Changes in Poisson's ratio produce a minor change in thermally induced stresses.

4. In situ stress ratio. A reduction in the horizontal to vertical stress ratio produces low compressive, to tensile, stresses in the roof and floor.

5. Canister locations. The two cases, (a) inclined double rows of canisters located in the floor, and (b) canisters located in the floor and side walls, both resulted in a more uniform distribution of thermal loads around the excavation compared to the base case. This uniform distribution of thermal load results in slight reduction in temperatures and rock stresses.

6. Room shape. Arched roof profile caused a reduction of stress concentrations in the roof-wall corners, but results in higher tangential stress at midspan. Circular rooms give rise to approximately equal all round tangential stress.

7. Room spacing. For reduced pillar width, shadowing of the central rooms from the high horizontal stresses was observed. This produced lower stresses in the roof and floor, but higher stresses in the side walls.

8. Canister placement sequence. For two-year delays in canister placement in adjacent rooms, thermal stresses for 5-year retrievability are only slightly less than the base case.

9. Retrievability period. The retrievability period has a major thermo-mechanical impact. Many of the above observations are different for 25- and 50-year retrievability periods because of significant interaction of adjacent rooms after five years. Only slight increases in maximum thermal tangential stresses around the rooms were noticed after an elapsed time of 25 years.

10. Ventilation. Maintaining the room air temperatures to 45°C for periods of 5 and 25 years results in significant quantities of heat being removed from the rock mass.

2.3 Regional Analysis

1. The age of spent fuel. The age of the spent fuel has a significant effect on the thermal profile above and below a repository. Five-year-old waste produces lower temperatures than the base case than ten-year-old waste for equivalent initial gross thermal loading.

2. Form of waste. Reprocessed high-level waste produces significantly lower temperatures and a faster temperature decay than spent fuel. A mixture of PWR and BWR spent fuel produces only minor changes from the base case.

3. Repository shape. The layout of panels of a full-scale repository can have a significant effect on long term temperatures and stress distributions. However up to 500 years one-dimensional analysis is adequate to determine temperature distributions above the center of these panels.

4. Sequencing. On the regional-scale delays of up to 20 years in canister placement have negligible impact on temperatures and stresses away from the level of the repository.

5. Heat transport in aquifers. Heat transfer in an overlying aquifer by forced convection can produce a negligible variation in temperatures above the repository. Flow in a flow top beneath the repository produced more significant temperature distortion. Flows of ten times the base flow significantly modify the temperature distribution around the repository.

6. Coupled thermal, fluid, and stress analyses of simplified stratigraphic sections were undertaken primarily to demonstrate the capabilities of the developed programs. From these preliminary analyses, the following tentative conclusions can be made. Induced buoyancy flow. Thermal gradients around the repository induce

upward groundwater motion which is dependent on the gross thermal loading. For a gross areal thermal loading of 25 W/m^2 , particles do rise vertically to the upper more permeable zones even with moderate regional cross flow.

7. Particle motion. Particle tracks in simulations indicate that the majority of fluid particles released from the repository level could rise vertically and then travel horizontally to the bottom of a permeable medium. Some of the particles appeared to move approximately 5000 meters horizontally for an elapsed time of 10,000 years.

8. Upper permeable zone. Zones of moderate permeability and porosity can act as significant retarders of fluid particle motion.

9. Coupled thermal fluid and stress. Stress and deformation changes do result in moderate changes in permeability and porosity. The changing of intrinsic hydraulic properties of the media with time does have an effect on particle motion.

3.0 DESCRIPTION OF BASE CASE FOR PARAMETER STUDY

A parametric study implies determination of the influence of an input parameter on the output function. For this study the input parameters include material properties of basalt and aquifer layers, geometric layouts of excavations and waste canisters, waste forms and age as well as such factors as retrievability periods, initial stress state, etc. The output factor in general is the repository performance in isolating the nuclear wastes in the short term during construction and emplacement and over the longer term when groundwater and radionuclide transport is important. More specifically for this parameter study the output functions are temperature and stresses.

For clarity in presentation of the parametric study a base set of parameters were selected. These represent realistic estimates of basalt properties, waste forms, stress fields, geometric layouts, etc., but do not represent a recommended repository layout.

The waste form used throughout is spent unprocessed fuel (SURF) from a pressurized water reactor. A typical canister has been chosen assumed to be 5 meters long and 0.4 m in diameter and contains 1 kilowatt of energy at the time of burial. The decay curve has been approximated as the sum of several exponential terms. The number of terms used depends on the time frame of interest. Section 6.2 lists the decay constants used.

The layout of the assumed room geometry is shown in Figure 3.1. The canisters are placed along the center line of the room floor with spacing such that the average initial gross thermal load is 25 W/m^2 . This results in canisters placed every 1.33 m. The assumed depth of the repository is 1000 m which is approximately the depth of the Umtanum flow, one possible candidate flow for the location of a repository.

FIGURE 3.1

EXCAVATION AND CANISTER LOCATION GEOMETRY, BASE CASE

The horizontal stress at depth has been assumed equal to the vertical stress (i.e., lithostatic conditions) and the thermal gradient was taken to be $0.04^{\circ}\text{C}/\text{m}$. No stress measurements have been recorded in the basalt flows to our knowledge, but in other parts of the U.S. stress measurements have shown a trend towards the lithostatic case at depths around 1000 m (Lindner and Halpern, 1977). The thermal gradient is compatible with borehole temperature measurements from the Hanford Site (see ARH-ST-137).

Rock properties are summarized in Table 3.1. These were selected after review of the report by Agapito, et al., 1977 and seem compatible with the recent laboratory studies made at the Colorado School of Mines, Duvall, et al., 1978.

TABLE 3.1
BASE GEOMETRY AND PROPERTIES

Rock and Waste Properties					
Material	Basalt	Sandstone	Waste	Concrete	Steel
Density (kg/m ³)	2900	1930	10,000	2240	7880
Diffusivity (m ² /sec)	6.5x10 ⁻⁷	2.3x10 ⁻⁷	7.1x10 ⁻⁷	3.4x10 ⁻⁷	1.12x10 ⁻⁵
Heat capacity (J/m ³ °C)	3.0x10 ⁶	1.9x10 ⁶	2.9x10 ⁶	2.240x10 ⁶	4.0x10 ⁶
Elastic modulus Pa	.48x10 ¹¹	NU	NU	NU	NU
Poisson's ratio	0.2	NU	NU	NU	NU
Thermal expansion coef.(1°C)	5.4x10 ⁻⁶	NU	NU	NU	NU
Permeability m/sec	1.0x10 ⁻⁹	1x10 ⁻⁶			
Porosity	5x10 ⁻⁴	0.10			
Canister geometry	Length	Diameter	Depth of Hole		
	5 m	0.4 m	8 m		
Room geometry	Width	Height	Spacing		
	6 m	7.5 m	24 m		
Depth of repository	1000 m				
Stress state:	Vertical	Horizontal			
	25 MPa	25 MPa			

NU - Not used.

4.0 CANISTER-SCALE THERMO-MECHANICAL RESPONSE

Stainless steel canisters containing spent Zircalloy hulls are to be placed in boreholes driven into the basalt. In order to determine the temperature rise within the canister and the surrounding rock, transient one-dimensional thermal calculations have been undertaken. The thermal properties of the radioactive waste, spent fuel elements and the canister have not been completely determined as yet; however, preliminary thermal properties of the waste material have been provided by Rockwell as follows: pure uranium, thermal conductivity of $2.09 \text{ J/sec m } ^\circ\text{K}$, specific heat of $293 \text{ J/kg } ^\circ\text{K}$ and a density of 10^4 kg/m^3 . A proposed geometrical layout for the excavations and canister locations is illustrated in Figure 4.1. This layout illustrates rooms with central boreholes driven into the floor and canisters located on a rectangular planar grid.

4.1 One Dimensional Analysis

The geometry as shown in Figure 4.1 was simplified so that one-dimensional thermal calculations could be undertaken. Since the canister is modelled as an infinitely long cylinder the one-dimensional analyses will only be applicable for short time frames. The calculations ignored end effects, etc.; however one-dimensional analyses do provide a simple means of undertaking parametric analyses and are applicable at a mid-height section of the canister for short elapsed times. The simplified one-dimensional geometry is illustrated in Figure 4.2. The one-dimensional thermal calculations were undertaken by the explicit finite difference program HEAT (see Appendix 1) and the finite element program DAMSWEL (Williams et al., 1977). In all of the analyses the thermal energy of the canister was 0.2 kW/m . The exterior boundary was a zero flux boundary as indicated in Figure 4.2. The outer radius of the problem domain was 4.4 meters, which was determined from an equivalent plan area for canisters

FIGURE 4.1

GEOMETRICAL ARRANGEMENT FOR CANISTER EMPLACEMENT
OF A SINGLE ROW OF CANISTERS IN A ROOM

FIGURE 4.2

SIMPLIFIED CANISTER GEOMETRY FOR ONE-DIMENSIONAL ANALYSES

located in a rectangular grid 2 x 30 meters.

4.2 Influence of Canister Thermal Properties

Since only preliminary thermal properties of the canister material have been provided at this time, it was considered worthwhile to investigate the influence of varying the canister thermal properties. The transient temperature distributions in the canister and basalt for the case of no air gap and reducing the canister thermal conductivity by a factor of two are illustrated as Cases A and B in Figure 4.3 for elapsed times of 0.5 and 1.0 year. There is no detectable difference in the basalt temperatures between Case A and B; however there is a slight increase in canister center line temperature for Case B compared to Case A.

4.3 Influence of Basalt Properties

Reducing the basalt thermal conductivity has a significant effect on the resulting temperature distributions in the canister and the basalt as is illustrated in Figure 4.4. Comparing the cases of A and C, thermal conductivity of basalt equal to 1.95 and 1.3 J/sec m $^{\circ}$ K respectively, the canister center line temperatures differ by 23 $^{\circ}$ C for 0.5 year and 21 $^{\circ}$ C for 1.0 year. The surrounding basalt temperatures are elevated for Case C compared with Case A by similar amounts. Thus, a reduction in the thermal conductivity of the basalt by 33% results in increasing the basalt and canister temperatures by approximately 20 $^{\circ}$ C for the geometry and configurations investigated here.

4.4 Influence of Air Gap/Borehole Decrepitation

The case of a complete air gap has not been investigated here; however, the cases of stagnant air voids in crushed basalt have been. A range of ratios of air voids present to total gap volume of 0, 0.5 and 0.8 have been

FIGURE 4.3

TRANSIENT TEMPERATURE DISTRIBUTIONS IN BASALT FOR
VARIOUS CANISTER CONDUCTIVITIES

FIGURE 4.4

TRANSIENT TEMPERATURE DISTRIBUTIONS FOR VARIOUS
CANISTER AND BASALT PROPERTIES WITH NO GAP

investigated. The case of zero air voids involves direct contact between the canister and the surrounding basalt. The transient distributions in the canister, crushed rock, and basalt are illustrated in Figure 4.4 for the case of no air gap, in Figures 4.5 and 4.6 for different gap widths. A stagnant air gap partially filled with crushed basalt acts like an insulator thus raising the temperature of the canister. An increase in gap width from 0.025 to 0.15 m with 80% air voids present resulted in an increased temperature rise at the canister center line of 40°C for an elapsed time of 1 year as shown in Figures 4.5 and 4.6. The boundary conditions for this problem illustrated in Figures 4.5 and 4.6 are the same as shown in Figure 4.2.

4.5 Borehole Decrepitation

The influence of changes in basalt thermal conductivity resulting from failure of the basalt were studied using the one-dimensional revision of STEALTH. Appendix 2 provides details of this study and only the highlights are presented here.

The coupling between thermal and mechanical response used for modelling the effects of borehole decrepitation was a volumetric strain-dependent thermal conductivity. This type of coupling is supported by the observation that, during rock failure, micro cracks and void spaces develop; i.e., the volumetric strain increases. The development of voids in the rock will lead to a reduced thermal conductivity, and hence restrict flow of energy from the canister to the rock.

Figure 4.7 shows the assumed thermal conductivity, volumetric strain relationship used in the analysis. The form shows a reduction in thermal conductivity to one quarter of the initial values for large volumetric strains. Also for compression volumetric strains the conductivity is unchanged.

FIGURE 4.5

TRANSIENT TEMPERATURE DISTRIBUTIONS IN BASALT
FOR VARIOUS GAP WIDTHS

FIGURE 4.6

TRANSIENT TEMPERATURE DISTRIBUTIONS WITHIN THE
CANISTER WITH VARIOUS GAP WIDTHS

FIGURE 4.7

FORM OF THERMAL CONDUCTIVITY - VOLUMETRIC STRAIN RELATIONSHIP

The analysis included an imposed far field stress of 28 MPa and a failure yield stress of 23 MPa so that failure occurred around the hole after heating was initiated. Figure 4.8 shows the volumetric strain after 28 days and the resulting thermal conductivity distribution. Notice that the thermal conductivity of the basalt dropped to 29% its initial value near the canister rock interface.

The results of the analyses are summarized in Figure 4.9, where the temperature change from the initial temperature of the basalt for the case with thermal/mechanical coupling is compared with the case with constant thermal conductivity. This shows that the reduced thermal conductivity of the rock adjacent to the canister causes an increase of 60% of the canister temperature at this time. This could be considered significant and indicates the potential for thermal runaway. Clearly further work is required on this problem and additional laboratory data are required to quantify the form at the thermal/mechanical coupling.

4.6 Borehole Lining

The spent fuel test associated with the Near-Surface Test Facility consists of the emplacement, monitoring, and retrieval of radioactive waste canisters. A schematic of the canister-borehole configuration to be used in these tests is shown in Figure 4.10. One objective of the tests is to determine the rate of heat loss up the borehole and into the test room. This factor is of interest because it will affect both the surrounding rock temperatures and the ventilation load of a full-scale repository.

An axisymmetric heat flow analysis of the canister-borehole configuration was performed to determine the effect of the liner thickness on the rate of heat loss. This analysis was performed with the computer code described in Appendix 4, with a simple one-dimensional conduction element used to represent

FIGURE 4.8

CONDUCTIVITY VERSUS RADIAL DISTANCE AFTER 28 DAYS

FIGURE 4.9

COMPARISON OF TEMPERATURES FOR UNIFORM CONDUCTIVITY (CASE A)
AND BASALT DECREPITATION (CASE B)

TEST ROOM FLOOR

STEEL REINFORCED
CONCRETE SHIELDING
PLUG WITH SUFFICIENT
STRENGTH TO SUPPORT
EMERGENCY EQUIPMENT

**NOMINAL
CANISTER
DIMENSIONS**
12.75" DIAMETER
14' LENGTH

FIGURE 4.10

SPENT FUEL CANISTER IN STORAGE HOLE

the borehole liner. The finite element mesh and location of the different materials used in the analysis are shown in Figure 4.11. The thermal properties of each material are summarized in Table 3.1. Note the high thermal conductivity of the steel relative to concrete and basalt. An 18°C initial temperature was given to all nodes, with the top boundary held at this temperature and the other boundaries having a no heat flow boundary condition. The canisters used in the tests will contain 4-year-old SURF having a power output at time of emplacement of 1.3 kw. Due to the short time span of the heat flow analysis, it was possible to represent this heat source with one exponentially decaying component having a half-life of 2.24 years. The air gap between the canister and the borehole wall was 0.1 m and was assumed to be stagnant (no convection).

The two cases of no liner and a steel liner of 0.03 m thickness were examined. Comparison of the resulting temperatures at four points near the liner show its effect on the heat flow. Figure 4.12 (a) is a comparison of the temperature at the top of the liner, Point A of Figure 4.11 (b). The presence of the liner causes a large temperature increase at Point A, with the difference about 15°C after 60 days. This increase would be expected, since the liner provides a thermal "connection" between the hot mid-height region of the canister and the cooler end region.

Figure 4.12 (b) and (c) plot temperature with and without the steel liner for Points B and C located in the concrete plug and basalt, respectively, near Point A. After 60 days the temperature difference is 4°C at B and only 2°C at Point C. This temperature difference seems unlikely to cause a significant change in heat loss up the borehole. The energy transfer to the ends of the liner should cause a temperature decrease at the middle of the liner. This decrease is shown in Figure 4.12(d) which is a temperature comparison of the

(a)

(b)

FIGURE 4.11 (a) AND (b)

FINITE ELEMENT MESH AND LOCATION OF MATERIALS USED IN AXISYMMETRIC ANALYSIS

FIGURE 4.12 (a) AND (b)

COMPARISON OF TEMPERATURE HISTORIES FOR AN UNLINED
AND LINED BOREHOLE, (a) POINT A, (b) POINT B

(See Figure 4.11 (b))

FIGURE 4.12 (c) AND (d)

COMPARISON OF TEMPERATURE HISTORIES FOR AN UNLINED

AND LINED BOREHOLE, (c) POINT C, (d) POINT D,

(See Figure 4.11 (b))

liner and no liner cases for Point D at mid-height of the canister but one liner radius into the basalt.

The main effect of the liner is to smooth out the temperature distribution along the borehole wall. The temperature profile along the borehole wall for both cases at times of 3, 30, and 60 days is plotted in Figure 4.13; the smoothing effect is clearly shown.

An overall picture of the differences in temperature distribution between the no liner and liner cases can be obtained from Figures 4.14 (a) and (b), which show the approximate temperatures at every node of the finite element mesh for $t = 60$ days. These plots emphasize the smoothing nature of the liner, and the insignificant heat loss up the borehole.

4.7 Summary of Canister-Scale Studies

In Table 4.1, the temperatures at the canister center line and borehole wall are quoted for various geometrical configurations and material properties variations. These temperatures were computed from one-dimensional and two-dimensional axisymmetric analyses with a canister thermal source of 0.2 kW/m for elapsed times of 0.5, 1, and 2 years. The decrepitation and borehole lining studies also shown in Table 4.1 were for 28 and 60 days, respectively. The borehole lining study was for a younger spent fuel (to model the spent fuel test facility under construction at Gable Mountain), so is not comparable to the other cases. It is apparent from a review of the temperatures shown in Table 4.1 that the canister temperature is very susceptible to the gap dimension or to the development of a zone of reduced basalt conductivity as might accompany basalt decrepitation. The exact modeling of the heat transfer between the canister and the basalt will include radiation

FIGURE 4.13
TEMPERATURE PROFILE ALONG LINER LOCATION,
POINTS A-E, FOR 3, 30, 60 DAYS

SYMBOL KEY

9	GE	90	} °C
8	GE	80	
7	GE	70	
6	GE	60	
5	GE	50	
4	GE	40	
3	GE	30	
2	GE	20	
1	LE	20

TIME=1440. HOURS

FIGURE 4.14 (a)

TEMPERATURE DISTRIBUTION FOR THE NO LINER CASE

(See Figure 4.11 for mesh)

SYMBOL KEY

9	GE	90	} °C
8	GE	80	
7	GE	70	
6	GE	60	
5	GE	50	
4	GE	40	
3	GE	30	
2	GE	20	
1	LE	20

TIME=1440. HOURS

FIGURE 4.14 (b)

TEMPERATURE DISTRIBUTION FOR THE 0.03 m LINER CASE

(See Figure 4.11 for mesh)

5.0 ROOM SCALE THERMO-MECHANICAL RESPONSE

The room scale studies involve the geomechanical modeling of the interaction of the heat generated by canister placement and the excavation. The primary objective of these studies was to establish acceptable waste disposal densities per room and to design size, shape and support requirements for these rooms. The thermo-mechanical analyses presented here are for two-dimensional plane geometry which assumes that the thermal output of the canisters can be modelled as uniformly distributed strip heat sources. The analyses were undertaken by the finite element programs FINEL (Hitchins, 1975), DAMSWEL (Williams, et al., 1977) and the boundary element program BEH2D, (Hocking, 1978).

A large number of parametric analyses have been undertaken in order to determine optimum size, shape and support of the rooms and canister location and placement sequence. Due to time constraints the parametric analysis is not a comprehensive one, but does provide data for establishing guidelines for room design. In order to avoid confusion the parametric studies have been conducted on a base case with the variation of only a single variable at any one time. Therefore this chapter has been subdivided into sections describing the effect each variable has on the base case. The methodology followed in this parametric study is illustrated diagrammatically in Figure 5.1. The geometry for the base case is illustrated in Figure 5.2 and the material properties, areal thermal loading, and in situ stress fields used for the base case are described in Chapter 3.0. Unless specifically stated otherwise the geometry, properties, areal thermal loading, and stress fields will be as mentioned in Chapter 3.0 throughout this chapter.

The thermal output from the radioactive waste canisters was represented

BASE CASE

- * Rectangular openings
- * Pillar width 24 m
- * Lithostatic stress field
- * Thermal loading 25 w/m^2
- * Retrievalability 5 years
- * Canisters in floor
- * Constant basalt properties
- * Depth 1000 m
- * No ventilation of rooms

DIFFERENT OPENING SHAPES

- * Arched roof
- * Circular cross section

REDUCED PILLAR WIDTHS

- * Pillar 12 m
- * Pillar 6 m

DIFFERENT STRESS FIELDS

- * HOR= 0.5 VER
- * HOR= 1.5 VER

INCREASED THERMAL LOADING

- * 50 w/m^2

DIFFERENT RETRIEVABILITY PERIODS

- * 25 years
- * 50 years

VARIOUS CANISTER LOCATIONS

- * Inclined vertical
- * In sidewalls

CHANGES IN BASALT PROPERTIES

- * Young's modulus
- * Poisson's ratio
- * Thermal expansion

INFLUENCE OF DEPTH

- * Increased depth

EFFECT OF VENTILATION

- * Rooms cooled

FIGURE 5.1SUMMARY OF PARAMETERS
VARIED IN ROOM-SCALE STUDY

FIGURE 5.2

BASE CASE FOR EXCAVATION AND CANISTER LOCATION GEOMETRY

by equation 5.1. The coefficients λ and Q are listed in Table 5.1.

$$Q_t = Q_i e^{-\lambda_i t} \quad (5.1)$$

where Q_t is the thermal power output of the canister at time t .

TABLE 5.1
COEFFICIENTS FOR THREE-COMPONENT EXPONENTIALLY DECAYING SOURCE

i	Proportion Q_i/Q_0	Decaying Constant λ
1	0.228	0.0533
2	0.614	0.0187
3	0.158	0.00138

5.1 Influence of Thermal Loading

The problem area for the room-scale thermo-mechanical analyses by the finite element programs FINEL and DAMSWEL is illustrated in Figure 5.3. This model is for an infinite number of parallel rooms (thus the reason for the lines of symmetry) and immediate canister placement in all rooms. The region of interest extends to the surface and to considerable depth below the rooms. A portion of the finite element mesh immediately around the rooms is illustrated in Figure 5.4. The finite elements in all of the analyses consisted of 8 noded isoparametric elements. The temperature distribution around the room for an elapsed time of 5 years is illustrated as contours in Figure 5.5. The plan areal thermal loading for this case was 25 W/m^2 as stated for the base case in Chapter 3.0. The air in the room was analyzed as if it were stagnant and no convection or radiation heat transfer mechanisms were modeled. The temperature contours are plotted in $^{\circ}\text{K}$. The ambient rock temperature at a depth of 1000 m in the basalt was assumed to be 340°K . The thermal stresses at various points in the basalt

FIGURE 5.3

PROBLEM AREA FOR THERMO-MECHANICAL FINITE ELEMENT ANALYSES

FIGURE 5.4

FINITE ELEMENT MESH FOR PLOTTED DATA

FIGURE 5.5

TEMPERATURE CONTOURS FOR ELAPSED TIME OF
5 YEARS - AREAL THERMAL LOADING OF 25W/m²

around the rooms are illustrated in magnitude and direction for this case in Figure 5.6. The magnitude of the stresses are measured between the ends of the crosses. Tensile stresses is denoted by arrowheads. Only thermal stresses are presented in this figure and no account of in situ stress fields has been considered. The most significant effect the thermal loading has on the resulting stress distribution is an increase in the horizontal stresses below the floor of the rooms. This is due to the confinement provided by the lines of symmetry.

The excavation and canister location geometry analyzed by the boundary element program BEH2D is illustrated in Figure 5.7. The number of rooms was limited to six in the boundary element analysis in order to investigate the effect of a finite number of parallel rooms. Except for the limited number of rooms the base case analyzed by the boundary element method is the same as mentioned in Chapter 3.0. The initial in situ field stresses were assumed to be 25 MPa (approximately 3,750 psi) at a depth of 1000 m (approximately 3,250 ft). The horizontal stress field was assumed equal to the vertical. The stresses and temperatures around the central room at an elapsed time of 5 years are shown in Figure 5.8. The initial boundary stresses are due to excavating the room in an existing stress field and do not include any thermal stresses. The boundary temperatures are in $^{\circ}\text{C}$ above the ambient temperature which at a depth of 1000 m was assumed to be 340°K . The total boundary stresses is a combination of the initial and thermal boundary stresses. The boundary stresses and temperatures are plotted perpendicular to the room boundary at the scale mentioned. Since there are no tractions applied to the boundary of the rooms, the boundary stresses plotted act in a direction parallel to the room boundaries. Thermal stress in the center

FIGURE 5.6

STRESSES FOR ELAPSED TIME OF 5 YEARS - AREAL
THERMAL LOADING OF 25W/m^2

FIGURE 5.7

EXCAVATION AND CANISTER LOCATION GEOMETRY
FOR BOUNDARY ELEMENT ANALYSES, BASE CASE

SCALES : 1CM NEPS 2.0 METRES 1CM NEPS 25. MPa 1CM NEPS 20. DEGS CENTIGRADE

FIGURE 5.8

BOUNDARY STRESSES AND TEMPERATURES FOR CENTRAL EXCAVATION

AT AN ELAPSED TIME OF 5 YEARS - 25 W/m² AT 1000m DEPTH

of the floor of the room was approximately 15 MPa (2250 psi) as computed by the boundary element program, Figure 5.8, and is in close agreement (to two significant figures) to the value computed by the finite element program. The boundary stresses and temperatures for one half of the right-hand edge room are illustrated in Figure 5.9. The stresses and temperatures for the central and edge room (Figures 5.8 and 5.9, respectively) are almost identical.

The base case was analyzed with an increased areal thermal loading of 50 W/m^2 . The boundary stresses and temperatures for an elapsed time of 5 years and at a depth of 1000 m are shown in Figure 5.10. The boundary stresses and temperatures for this case, Figure 5.10, are significantly larger than for the base case, Figure 5.8. The variation of boundary stress with areal thermal loading for the particular geometry and properties as given in the base case is plotted in Figure 5.11 for three boundary points. The basalt in the floor of the room is subjected to the greatest increase in stress due to the thermal loading at an elapsed time of 5 years. The boundary stress at the center of the floor increases from 24 MPa (approximately 3150 psi) to 51 MPa (approximately 7650 psi) for areal thermal loadings from 0 to 50 W/m^2 , respectively.

5.2 Influence of Depth

The initial in situ stress field was assumed to be lithostatic with a value of 25 MPa (3750 psi) at a depth of 1000 m (3,250 ft). Increasing the depth at which the rooms are to be excavated will result in an increase in the initial in situ stress field. The boundary stresses and temperature for the base case at a depth of 1400 m are illustrated in Figure 5.12. The variation of boundary stresses (with and without thermal stresses) for three

FIGURE 5.11

EFFECT OF AREAL THERMAL LOADING ON BOUNDARY
STRESSES FOR THE BASE CASE

SCALES : 1CM NEPS 2.0 METRES 1CM NEPS 25. MPa 1CM NEPS 20. DEGS CENTIGRADE

FIGURE 5.12

BOUNDARY STRESSES AND TEMPERATURES FOR CENTRAL EXCAVATION
AT AN ELAPSED TIME OF 5 YEARS - 25 W/m² AT 1400m DEPTH

points are plotted against depth in Figure 5.13. The variation of boundary stresses with depth is linear, since the analyses undertaken in this section assumed linear elastic behavior of the basalt rock mass, and a linear increase in the in situ stress field with depth.

5.3 Influence of Basalt Properties

The variation in boundary stresses for the three points A, B, and C due to changes in basalt properties, Poisson's ratio, Young's modulus, and coefficient of linear thermal expansion are illustrated in Figure 5.14 from the base case. A reduction of Poisson's ratio from 0.2 to 0.1 results in a reduction of the thermal stresses by 11%. The thermal stresses vary linearly with both Young's modulus and the coefficient of linear thermal expansion; that is, half the modulus or expansion coefficient results in halving the thermal stresses. The boundary stresses illustrated in Figure 5.14 are for an areal thermal loading of 25 W/m^2 and a horizontal field stress of 25 MPa equal to the vertical field stress. The boundary stresses due to excavating the rooms, that is zero thermal stresses, are independent of the elastic parameters of the basalt and are therefore not affected by any variation in basalt elastic properties.

5.4 Influence of In Situ Stress Ratios

The boundary stresses and temperatures with initial in situ field stresses of horizontal = 12.5 MPa (1875 psi) and vertical = 25 MPa (3750 psi) are illustrated in Figures 5.15 and 5.16 for the central and edge room respectively. The most significant difference between this case and the base case shown in Figure 5.8 is the much reduced initial boundary stresses in the roof and floor. In fact very slightly tensile stresses are present in

FIGURE 5.13

EFFECT OF DEPTH ON EXCAVATION BOUNDARY STRESSES FOR BASE CASE

FIGURE 5.14

EFFECT OF BASALT THERMO-MECHANICAL PROPERTIES ON
STRESSES FOR THE BASE CASE

SCALES : 1CM REPS 2.0 METRES 1CM REPS 25. MPa 1CM REPS 20. DEGS CENTIGRADE

FIGURE 5.15

BOUNDARY STRESSES AND TEMPERATURES FOR CENTRAL
EXCAVATION WITH INITIAL FIELD STRESSES OF HOR = 0.5 VER

SCALES : 1CM NEPS 2.0 METRES 1CM NEPS 25. MPa 1CM NEPS 20. DEGS CENTIGRADE

FIGURE 5.16

BOUNDARY STRESSES AND TEMPERATURES FOR EDGE EXCAVATION
WITH INITIAL FIELD STRESSES OF HOR = 0.5 VER

the roof and floor for the case of zero thermal loading. The total boundary stress (including thermal) is tensile in the roof for this case. For the case of initial in situ horizontal stress field 1.5 times the vertical, that is 37.5 MPa (5625 psi) and 25 MPa (3750 psi) respectively, the boundary stresses and temperatures are given in Figures 5.17 and 5.18 for the central and edge rooms. The boundary stresses are much higher in the roof and floor of the room for this case compared to the base case. The boundary stresses in the sidewalls are lower than the base case.

The variation of boundary stresses at three points on the boundary are shown in Figure 5.19 for various horizontal to vertical in situ stress field ratios at a depth of 1000 m for the central room. The boundary stresses in both the roof and floor of the room decrease with decreasing horizontal to vertical in situ stress field ratio, while the boundary stress in the sidewall increases with decreasing vertical stress ratio.

5.5 Influence of Canister Locations

Two alternative configurations of canister locations were analyzed to determine the influence of canister position on room performance. One of these alternative layouts of canister locations is illustrated in Figure 5.20. In this case the canisters are placed in boreholes inclined at 30° to the vertical. The canister boreholes could be either staggered down the length of the rooms or located directly opposite each other. Except for the canister locations, material properties, areal thermal loadings, stress fields, etc. are identical to the base case. The boundary stresses and temperatures for this case of alternative canister locations are illustrated in Figure 5.21.

The second alternative location of canisters is illustrated in Figure 5.22. In this case the canisters are located in the floor and sidewalls of the room.

FIGURE 5.17

BOUNDARY STRESSES AND TEMPERATURES FOR CENTRAL EXCAVATION
WITH INITIAL FIELD STRESSES OF HOR = 1.5 VER

SCALES : 1CM REPS 2.0 METRES 1CM REPS 25. MPa 1CM REPS 20. DEGS CENTIGRADE

FIGURE 5.18

BOUNDARY STRESSES AND TEMPERATURES FOR EDGE EXCAVATION
WITH INITIAL FIELD STRESSES OF HOR = 1.5 VER

FIGURE 5.19

EFFECT ON IN SITU FIELD STRESS RATIO ON BOUNDARY
STRESSES FOR BASE CASE

FIGURE 5.20

ALTERNATIVE LAYOUT OF RADIOACTIVE WASTE CANISTERS

BOUNDARY STRESSES INITIAL

BOUNDARY TEMPERATURES

BOUNDARY STRESSES TOTAL

SCALES : 1CM REPS 2.0 METRES 1CM REPS 25. MPa 1CM REPS 20. DEGS CENTIGRADE

FIGURE 5.21

BOUNDARY STRESSES AND TEMPERATURES FOR ALTERNATIVE CANISTER LOCATION

FIGURE 5.22

SECOND ALTERNATIVE LAYOUT OF RADIOACTIVE WASTE CANISTERS

The boundary stresses and temperatures for this case are illustrated in Figure 5.23. The boundary stresses and temperatures for the two alternative cases of canister location are plotted along with the base case in Figure 5.24. The significant differences between the two alternative canister configurations and the base case are the reduced temperatures in the floor and the reduced stresses in the sidewalls. This difference is due to the thermal loading being more evenly distributed around the room in the alternate configurations as compared to the base case.

5.6 Influence of Room Shape

Two alternative room shapes were considered in the study, (a) base case with arched roof and (b) circular room cross section. The arched roof room shape is illustrated in Figure 5.25. The difference between this room shape with arched roof and the base case is a slight increase in height and a curved roof. Except for the change in shape of the room this case is the same as the base case. The boundary stresses and temperatures for this alternative room shape are shown in Figure 5.26. The most significant feature of this alternative shape compared to the base case is the increased boundary temperatures do not appear to be significantly different from the base case. The circular room cross section with canisters located in the floor is shown in Figure 5.27. The boundary temperatures and stresses for this case are illustrated in Figure 5.28. The same excavation geometry was also analyzed except with canisters located in both the floor and sidewalls of the room, Figure 5.29. The stresses and temperature distributions around the rooms are illustrated in Figure 5.30.

SCALES : 1CM REPS 2.0 METRES 1CM REPS 25. MPa 1CM REPS 20. DEGS CENTIGRADE

FIGURE 5.23

BOUNDARY STRESSES AND TEMPERATURES FOR SECOND ALTERNATIVE CANISTER LOCATION

FIGURE 5.24

COMPARISON OF STRESSES AND TEMPERATURES FOR BASE
 CASE AND ALTERNATIVE CANISTER CONFIGURATIONS

FIGURE 5.25

ALTERNATIVE EXCAVATION SHAPE - ARCHED ROOF

SCALES : 1CM NEPS 2.0 METRES 1CM NEPS 25. MPa 1CM NEPS 20. DEGS CENTIGRADE

FIGURE 5.26

BOUNDARY TEMPERATURES AND STRESSES FOR
ALTERNATIVE EXCAVATION SHAPE - ARCHED ROOF

FIGURE 5.27

ALTERNATIVE EXCAVATION SHAPE - CIRCULAR

BOUNDARY STRESSES INITIAL

BOUNDARY TEMPERATURES

BOUNDARY STRESSES TOTAL

SCALES : 1CM REPS 2.0 METRES

1CM REPS 25. MPa

1CM REPS 20. DEGS CENTIGRADE

FIGURE 5.28

BOUNDARY STRESSES AND TEMPERATURES FOR CIRCULAR EXCAVATION SHAPE

FIGURE 5.29

CIRCULAR EXCAVATION WITH CANISTERS IN FLOOR AND WALLS

SCALES : 1CM REPS 2.0 METRES 1CM REPS 25. MPa 1CM REPS 20. DEGS CENTIGRADE

FIGURE 5.30

BOUNDARY STRESSES AND TEMPERATURES FOR CIRCULAR
EXCAVATION WITH CANISTERS IN FLOOR AND WALLS

5.7 Influence of Room Spacing

The geometry of a system of rooms and canister locations with a reduced pillar width from the base case is shown in Figure 5.31. The pillar width is reduced from 24 m for the base case to 12 m in this reduced room spacing geometry. The boundary stresses and temperatures for this case are illustrated in Figure 5.32. Another analysis was undertaken on the case of a further reduction in pillar width to 6 m, as shown in Figure 5.33. The temperature and stress distributions around a room for a pillar width of 6 m are illustrated in Figure 5.34. The tangential stresses at three points for the base case and the two previously mentioned reduced room spacing geometries (pillar widths of 12 and 6 m) are compared in Figure 5.35. The boundary stresses increase significantly at pillar mid-height for the case of a 6-m-wide pillar.

5.8 Influence of Canister Placement Sequence

The delayed placement of canisters from the central room to the edge room is shown in Figure 5.36. For the purpose of determining the influence of delayed placement of canisters, a two-year delay between the filling of two rooms and completion of two previous rooms was considered here. The boundary stresses and temperatures for the central room are illustrated in Figure 5.37 for an elapsed time of 9 years since the central rooms were filled. The boundary stresses and temperatures around the central room are not significantly different from the base case for similar elapsed times (see the following section).

5.9 Influence of Retrievability Period

The retrievability period has a significant bearing on areal thermal loading, room stability, etc. For the sake of determining this influence,

FIGURE 5.31

GEOMETRY FOR THE 12-METER ROOM SPACING

SCALES ■ 1CM REPS 2.0 METRES 1CM REPS 25. MPa 1CM REPS 20. DEGS CENTIGRADE

FIGURE 5.32

BOUNDARY STRESSES AND TEMPERATURES FOR
THE 12-METER ROOM SPACING CASE

FIGURE 5.33

GEOMETRY FOR THE 6-METER ROOM SPACING

BOUNDARY STRESSES INITIAL

BOUNDARY TEMPERATURES

BOUNDARY STRESSES TOTAL

SCALES : 1CM REPS 2.0 METRES

1CM REPS 25. MPa

1CM REPS 20. DEGS CENTIGRADE

FIGURE 5.34

BOUNDARY STRESSES AND TEMPERATURES FOR THE

6-METER ROOM SPACING

FIGURE 5.35

EFFECT OF ROOM SPACING ON BOUNDARY STRESSES

FIGURE 5.36
SEQUENCE OF CANISTER PLACEMENT FROM
CENTRAL TO EDGE ROOMS

SCALES : 1CM NEPS 2.0 METRES 1CM NEPS 25. MPa 1CM NEPS 50. DEGS CENTIGRADE

FIGURE 5.37
BOUNDARY TEMPERATURES AND STRESSES FOR
CANISTER PLACEMENT SEQUENCE

retrievability periods of 25 and 50 years were analyzed for: (a) the base case; (b) base case with alternative canister locations; (c) rooms of circular cross section.

The boundary stresses and temperatures around the central room for the base case at an elapsed time of 25 years are illustrated in Figure 5.38 as determined by the boundary element method. The temperature contours and thermal stresses computed by the finite element method are shown in Figures 5.39 and 5.40 respectively. The stresses illustrated in Figure 5.40 are purely thermal stresses and do not include the in situ field stresses.

The tangential stresses and boundary temperatures for the base case at an elapsed time of 50 years are illustrated in Figure 5.41. The stresses and temperatures for the alternate canister configuration at elapsed times of 25 and 50 years are shown in Figures 5.42 and 5.43 respectively. The analysis of circular rooms with radioactive waste canisters located in the floor was undertaken and the resulting stresses and temperatures are shown in Figures 5.44 and 5.45 for elapsed times of 25 and 50 years respectively. The tangential stresses for each of the configurations analyzed for elapsed times of 5, 25 and 50 years are illustrated in Figures 5.46, 5.47, and 5.48 for the base case, alternative canister locations, and rooms of circular cross section.

5.10 Influence of Ventilation

The base case was analyzed by the finite element method for the case where the rooms are ventilated. The room periphery was maintained at 320°K (47°C) throughout the analysis. The temperature distributions around the room at 5 and 25 years elapsed years are illustrated as contours in Figures 5.49 and 5.50 respectively. This level of ventilation gives rise to a large

FIGURE 5.38

BOUNDARY STRESSES AND TEMPERATURES AROUND THE
CENTRAL ROOM FOR AN ELAPSED TIME OF 25 YEARS

FIGURE 5.39
TEMPERATURE CONTOURS FOR BASE CASE AT AN
ELAPSED TIME OF 25 YEARS

FIGURE 5.40

STRESSES FOR BASE CASE AT AN ELAPSED TIME OF 25 YEARS

FIGURE 5.41

BOUNDARY STRESSES AND TEMPERATURES FOR BASE CASE AT AN ELAPSED TIME OF 50 YEARS

FIGURE 5.42

BOUNDARY STRESSES AND TEMPERATURES FOR FIRST
ALTERNATE CANISTER LOCATION, AFTER 25 YEARS

FIGURE 5.43

BOUNDARY STRESSES AND TEMPERATURES FOR FIRST
ALTERNATE CANISTER LOCATION, AFTER 50 YEARS

SCALES : 1CM REPS 2.0 METRES 1CM REPS 25. NPA 1CM REPS 50. DEGS CENTIGRADE

FIGURE 5.44

BOUNDARY STRESSES AND TEMPERATURES FOR CIRCULAR
EXCAVATION, AFTER 25 YEARS

SCALES : 1CM REPS 2.0 METRES 1CM REPS 25. MPa 1CM REPS 50. DEGS CENTIGRADE

FIGURE 5.45

BOUNDARY STRESSES AND TEMPERATURES FOR
CIRCULAR EXCAVATION, AFTER 50 YEARS

FIGURE 5.46

EFFECT OF RETRIEVABILITY PERIOD ON BOUNDARY STRESSES

FOR THE BASE CASE

FIGURE 5.47

EFFECT OF RETRIEVABILITY PERIOD ON BOUNDARY STRESSES
FOR ALTERNATIVE CANISTER LOCATION

FIGURE 5.48

EFFECT OF RETRIEVABILITY PERIOD ON BOUNDARY STRESSES
FOR CIRCULAR EXCAVATION

FIGURE 5.49

TEMPERATURE CONTOURS AFTER 5 YEARS, ROOM
TEMPERATURE 320 DEGREES KELVIN

FIGURE 5.50

TEMPERATURE CONTOURS AFTER 25 YEARS, ROOM
TEMPERATURE 320 DEGREES KELVIN

withdrawal of heat from the room; this point is clearly illustrated in the two figures. In this analysis a surface heat transfer coefficient between air and the basalt rock mass was not modeled. Analysis incorporating surface heat transfer elements is presently under way.

5.11 Summary of Room-Scale Studies

Table 5.2 presents a summary of the boundary stresses for the three points around a room heated from below for all cases analyzed in this section. In general the higher stressed cases indicate that a lower thermal loading is required so that a critical stress level is not exceeded. However this rule is not true for all cases as stability is sometimes higher, say for the circular or arched roof cases, even though high compressive stresses exist. Section 8.0 reviews the implication of these stress levels, in conjunction with the canister- and regional-scale studies, on the recommended allowable gross thermal loadings.

TABLE 5.2

COMPARISON OF BOUNDARY STRESSES AT SELECTED POINTS FOR VARIOUS CONFIGURATIONS AND LOADINGS

Condition	Location		
	Tangential room stress (MPa)		
	A*	B*	C*
Base Case	19.5	26.6	34.9
Thermal loading 50 W/m ²	19.6	32.0	50.3
Depth 1400 M	27.3	35.1	42.6
E = Twice base case	19.8	32.0	51.4
Poisson's ratio 0.3	19.7	27.0	36.8
" " 0.1	19.5	25.9	33.2
In-situ Horizontal 0.5 vert	0.7	36.0	14.7
" " 1.5 vert	39.7	17.3	55.1
Room Spacing			
12 m wide pillar	17.4	29.5	28.5
6 m wide pillar	10.2	45.7	22.0
Canister location
24.8	19.9	31.0
36.2	13.1	42.7
Room shape
64.2	30.0	34.1
55.7	65.1	71.9
81.0	43.1	87.8
Canister placement sequence	23.8	26.3	41.2
Retrievability 25 years
40.9	20.4	54.5
55.0	10.1	61.2
94.7	61.0	109.6
Retrievability 50 years
45.1	20.7	54.3
54.3	14.8	58.6
101.7	64.5	111.6

*Note: For location of points A, B and C see Figure 5.11

6.0 REGIONAL THERMO-MECHANICAL STUDIES

6.1 Introduction

Regional long-term effects resulting from waste emplacement in basalt at a depth of 1000m was studied using one-, two-, and three-dimensional models. The influence of spent fuel age and reprocessed waste on temperature changes above and below the repository was investigated using a one-dimensional code. To study the influence of repository shape and canister placement sequence a three-dimensional model was used. A preliminary analysis of the influence of groundwater flow in the Vantage Sandstone on the temperature distribution above the repository is presented using a two-dimensional explicit finite element code. Where possible a number of runs reflecting a range of inputs were made so that the influence of particular parameters could be identified.

6.2 Waste Form and Age

6.2.1 Background

To illustrate the influence of waste form and age on regional temperature changes the one-dimensional finite difference DIFFUS2 was used. This code is appropriate for analyses where all heat flow is either up or down away from the level of the canister placement. This is approximately the case at the center of a large repository where the lateral extent is significantly greater than its depth. Appendix 3 describes DIFFUS2 in detail.

Using DIFFUS2 the following types of waste form were used:

1. Spent unprocessed fuel, 10 years old (base case);
2. Spent unprocessed fuel, 5 years old;
3. Spent unprocessed fuel, 20 years old;
4. High-level waste (HLW), reprocessed;
5. Mixed PWR, BWR spent unprocessed fuel.

Figure 6.1 shows the heat generation rate for types 1, 2 and 3 and Figure 6.2 shows the corresponding curves for 1, 4 and 5. Table 6.1 lists the exponentially decaying components used to represent each of the waste forms.

These waste forms have different decay rates and hence a different initial gross thermal loading will be allowed for each waste form. The following analysis shows the different thermal histories that will develop in the basalt assuming an initial gross thermal loading of 25 W/m^2 for all cases. Other temperature profiles for different gross thermal loadings could be developed by linearly scaling the temperature in proportion to the initial gross thermal loading.

The hypothetical geological cross section assumed for this analysis consisted of basalt up to 240m from the surface, with sandstone to the surface. The thermal properties are listed in Table 6.2.

TABLE 6.2
THERMAL PROPERTIES USED IN REGIONAL ONE-DIMENSIONAL STUDIES

Property	Basalt	Sandstone
Thermal conductivity $\text{W/m}^\circ\text{C}$	1.86	0.46
Specific heat $\text{J/kg}^\circ\text{C}$	1030	1030
Density kg/m^3	2900	1930

6.2.2 Age

Figures 6.3 through 6.5 show the temperature profiles from the surface down through the repository and beyond for 10, 5 and 20 year old spent fuel. Shown in each figure are the temperatures at 50, 500 and 5000 years after heater emplacement. Figures 6.6 through 6.8 show temperature histories for three points above the repository. These points are respectively 25m, 200m,

FIGURE 6.1

COMPARISON OF THE HEAT GENERATION CURVES OF
DIFFERENT AGE SPENT UNREPROCESSED FUEL WASTES

FIGURE 6.2

COMPARISON OF THE HEAT GENERATION CURVES OF
DIFFERENT WASTE FORMS

TABLE 6.1

PROPORTION AND HALF-LIFE OF THE EXPONENTIALLY DECAYING SOURCE COMPONENTS

	5-Year-01d		PWR SURF 10-Year-01d		20-Year-01d		PWR HLW 10-Year-01d		2:1 MIX PWR: BWR SURF 10-Year-01d	
	Proportion	$t_{1/2}$ (YRS)	Proportion	$t_{1/2}$ (YRS)	Proportion	$t_{1/2}$ (YRS)	Proportion	$t_{1/2}$ (YRS)	Proportion	$t_{1/2}$ (YRS)
Q1	0.00449	30140	0.00756	30140	0.01014	30140	0.0002	46210	0.000556	1.73×10^6
Q2	0.2786	6970	0.0151	6970	0.0203	6970	0.0000688	9254	0.01095	20877
Q3	0.03659	396	0.1404	396	0.1852	396	0.0302	6189	0.0143	5001
Q4	0.4478	32	0.677	32	0.7313	32	0.0071	296	0.1366	408
Q5	0.0366	17.2	0.0504	17.2	0.0452	17.2	0.853	28.6	0.0157	128
Q6	0.2786	2.38	0.1093	2.38	0.00794	2.38	0.0778	5.92	0.599	33.8
Q7	0.1394	0.71	--	--	--	--	0.0649	1.44	0.137	16.1
Q8	--	--	--	--	--	--	--	--	0.0852	1.75

FIGURE 6.3

TEMPERATURE PROFILES DUE TO 10-YEAR-OLD SURF

FIGURE 6.4

TEMPERATURE PROFILES DUE TO 5-YEAR-OLD SURF

FIGURE 6.5

TEMPERATURE PROFILES DUE TO 20-YEAR-OLD SURF

FIGURE 6.6

TEMPERATURE HISTORY AT THREE POINTS ABOVE THE REPOSITORY HORIZON FOR 10-YEAR OLD SURF

FIGURE 6.7

TEMPERATURE HISTORY AT THREE POINTS ABOVE THE REPOSITORY HORIZON FOR 5-YEAR OLD SURF

FIGURE 6.8

TEMPERATURE HISTORY AT THREE POINTS ABOVE THE
REPOSITORY HORIZON FOR 20-YEAR-OLD SURF

and 400m above the repository level. The two later profiles correspond approximately to the levels of the Vantage Sandstone and Mabton Interbed.

The difference in these three cases is obvious. The 5-year-old waste has a significant proportion of heat-generating material with a short half-life; whereas for the 20-year-old waste these components are reduced to insignificant levels. Although the initial gross thermal loading for all three cases was the same, more energy is input to the basalt by 20-year-old waste, resulting in higher temperatures. To attain the same maximum temperature at 25m above the repository, the allowable gross thermal loadings for 5- and 20 year old waste would be 153 and 80 kw/acre, respectively (100 kw/acre $\approx$ 24.7 W/m²).

Table 6.3 summarizes the comparison of gross thermal loading for the various fuel ages. Because the initial thermal output of a 5-year-old canister is twice that of a 10-year-old canister, fewer 5-year-old canisters can be placed per unit area in order to achieve the same temperature above the repository. However the difference in canister loading density for 10 and 20-year-old waste is negligible.

TABLE 6.3

RELATIVE ALLOWABLE GROSS THERMAL LOADING AND CANISTER DENSITY
FOR DIFFERENT AGE SPENT FUEL

Spent Fuel Age (yrs)	Relative Initial Power Output	Relative GTL	Relative Number of Canisters Per Unit Area
5	2.00	1.53	0.765
10	1.00	1.00	1.00
20	0.82	0.80	0.98

6.2.3 Waste form

Waste forms could vary depending on recycling capabilities and nuclear plant design. Two forms of generating plants presently exist in the U.S. The Pressurized Water Reactor, PWR, and the Boiling Water Reactor, BWR, each have slightly different fuel rods which are left for differing periods within the reactor and hence produce different heat-generating waste materials. Re-processing and recycling the uranium and/or plutonium in various mixtures with fresh uranium feed produces other waste product forms. Figure 6.2 shows the heat-generating histories of three waste forms. These are PWR spent fuels, reprocessed high-level waste and a mixture of spent fuel from both PWR and BWR fuel assemblies. The difference between PWR and the mixed spent fuel is only marginal although the high-level waste differs significantly. The long half-life components of the spent fuel are missing from the high level waste.

Figures 6.9 and 6.10 show the temperature profiles for the mixed spent fuel and the high-level waste. These curves should be compared with the "base" case shown in Figure 6.3. Figure 6.9 is very similar to 6.2 whereas for the high level waste the temperatures are much lower. Figures 6.11 and 6.12 show the temperature histories for points 25, 200 and 400 meters above the repository. Again, the mixed PWR and BWR response is very similar to the PWR spent fuel (Figure 6.6) whereas the HLW shows much reduced temperatures.

To produce the same maximum temperatures in the basalt 25m above the repository level for the three waste forms the initial gross thermal loading must be changed. The allowable gross thermal loading for the mixed PWR:BWR and HLW would be 96 and 152 kw/acre, respectively.

FIGURE 6.9

TEMPERATURE PROFILES DUE TO 2:1 MIX, PWR:BWR SURF

FIGURE 6.10

TEMPERATURE PROFILES DUE TO HIGH-LEVEL WASTE

FIGURE 6.11

TEMPERATURE HISTORY AT THREE POINTS ABOVE THE REPOSITORY HORIZON
FOR 2:1 MIX, PWR:BWR SURF

FIGURE 6.12

TEMPERATURE HISTORY AT 3 POINTS ABOVE THE REPOSITORY HORIZON
FOR HIGH-LEVEL WASTE

6.3 Repository Shape and Sequencing

Regional studies of stress and temperature changes resulting from heat-generating waste emplacement at depths of 1000 meters below surface were performed. The object of these studies was to determine if repository shape would significantly influence temperatures, stresses, or displacements within the zone where shafts and service facilities would be located.

The analysis was by superposition of point heat sources placed in the floor of the repository in an infinite elastic material. The influence of the ground surface, a stress-free plane of constant temperature, was incorporated by superposition of equal but opposite strength sources in the mirror image position about the ground surface. The program used for this study has been used for other Rockwell projects--see Appendices 2 and 3 of our Phase I report--and was developed specifically for nuclear waste repository design work (St. John, 1977).

Three basic repository shapes were analyzed as shown in Figure 6.13. Up to 100 point heat sources were used to model the distributed effect of the canisters. In all analyses the base case 10-year-old spent fuel was assumed for the waste material. A three-component source was used to model the decay of the heat sources out to 500 years as shown in Table 6.4. Figure 6.14 shows a comparison of the three-component heat-generation curves with the actual heat generation rates. The correspondence to 500 years is within 4% at all times.

TABLE 6.4

THREE-COMPONENT EXPONENTIALLY DECAYING SOURCE
USED IN SHAPE AND SEQUENCE ANALYSIS

	Proportion	Half-Life (Years)	Decay Constant (Years ⁻¹)
1	0.228	13	0.0533
2	0.614	37	0.0187
3	0.158	500	0.00138

FIGURE 6.13

REPOSITORY GEOMETRIES CONSIDERED DURING THE
SHAPE AND SEQUENCE ANALYSIS

FIGURE 6.14
COMPARISON OF THREE-COMPONENT SOURCE WITH
ACTUAL HEAT-GENERATION RATE

6.3.1 Repository Shape

A total of five repository shapes was analyzed. The three shapes shown in Figure 6.13 were augmented by repositories similar to the two shapes but with the separation between the two or four waste areas (shown as S in the figure) reduced to 400 meters instead of 800 meters. The waste form used for these analyses was the 10-year spent fuel with only three exponential components used to represent the heat generation curve out to 500 years (see Table 6.4).

Some results from these analyses are shown in Figure 6.15 where the stress profiles above the center of the repository are plotted. All plots are for 500 years after placement of canisters. The location of the stress profiles in Figure 6.15 could correspond to shaft locations and service areas. Obviously a shaft pillar area would be required in which no heat sources would be located; this is not shown in the base case. Clearly when a shaft pillar is not left high compressive stresses near the repository level and reduced horizontal stresses above the repository could cause significant problems. However over the short term; i.e. the operating life of the shaft, say up to 50 years, these effects are small.

Figure 6.16 shows the stress profiles at other points above the various repository shapes. The stress changes are in general small with little interaction from the separated sections of the repository.

(a)

(b)

FIGURE 6.15

STRESS PROFILES ABOVE CENTER POINT A OF ALL GEOMETRIES

(a)

(b)

FIGURE 6.16

STRESS PROFILES ABOVE POINTS B OF ALL GEOMETRIES

Figure 6.17 shows a comparison of the temperatures above the repositories and the results from the one-dimensional DIFFUS2 code. Notice that for the three-dimensional cases the temperatures are nearly identical above the center of the heated areas, but significantly lower toward the periphery. The temperature influence after 500 years extends about 400 meters above the repository; this is still small relative to the lateral extent of the repository, hence the one-dimensional and three-dimensional solutions correspond.

6.3.2 Sequencing

The impact of sequencing canister placement was modelled very crudely by assuming that half the repositories were filled at time zero and that the remaining half filled after 20 years. Figure 6.13 shows the various sections filled at time zero and time 20. No results are presented from these analyses because on the time and geometric scale of the regional analyses such short-term details have no detectable effect. Sequencing would be important on the room or canister scale, or if the delay between filling two sections was of the order of hundreds of years.

6.4 Heat Transfer by Forced Convection in Interbeds and Flow Tops

An interbed such as the Vantage Sandstone above and flow tops above or below the repository level could be regions of greater groundwater flow relative to the more impermeable basalt flows. To assess the impact of these zones on heat transfer and subsequent thermal stresses, two series of analyses were performed. In the first series, the convective heat transfer was restricted to two thin aquifers positioned to approximate the Vantage and Mabton Interbed; in the second, a third hypothetical aquifer was introduced below the repository. The third aquifer could represent a zone of fractured basalt associated with a flow top located near the repository.

(a)

(b)

FIGURE 6.17

TEMPERATURE PROFILES ABOVE POINTS A, B, AND C
OF ALL GEOMETRIES, (a) 2 LOBE, (b) 4 LOBE

All aquifers were assumed to be 4m thick. A more detailed description of the hydrology of the Hanford Site is presented in Section 7.0 and is based on LaSala and Doty (1971). Appendix 4 provides technical details of the analysis technique used and the runs performed.

The geologic section modelled was the same as for the one-dimensional analysis presented in Section 6.2 and the waste form was the 10-year-old spent unprocessed fuel. A two-dimensional finite element model was used: in the first series only half of the repository being modelled. The problem is not completely symmetrical because the lateral groundwater flow through the aquifers causes temperature decreases to the left of the problem and temperature increases to the right. However for a limited time period the geometric center line is a line of no heat flux. The cases run in the first series approximated this no flux condition. In the second series with the lower aquifer included a more extensive mesh was used so that the no flux condition of the repository center line was not a restriction.

Three analyses were performed to illustrate the influence of varying flow rate in the aquifers on the temperature distribution. One case had no flow, the second base case had flow velocity in the sandstone of 1×10^{-7} m/sec, and the third flow was taken as 10 times the base flow. For all runs, all other parameters were held constant.

Figures 6.18, 6.19, and 6.20 show 5000-year temperature contours for the three cases for the first series of analysis. It is clear that for the base flow only very marginal changes are evident in the temperature distribution. But the base flow times ten case shows significant disturbance to the temperature contours (Figure 6.20). Table 6.5 lists the length of aquifer above the repository in which the temperature change exceeds 15°C , 30°C , and 40°C after

TEMPERATURE CONTOURS FOR TIME= 5000. YEARS

TEMPERATURE CONTOURS FOR TIME= 5000. YEARS

Horizontal and Vertical
Scales Are Equal

FIGURE 6.18

FIGURE 6.19

TEMPERATURE CONTOURS (DEGREES CENTIGRADE)

TEMPERATURE CONTOURS (DEGREES CENTIGRADE)

FOR THE NO FLOW CASE AT 5000 YEARS

FOR THE 1×10^{-7} METERS PER SECOND BASE FLOW CASE AT 5000 YEARS

FIGURE 6.20

TEMPERATURE CONTOURS (DEGREES CENTIGRADE)

FOR THE 1×10^{-6} M/SEC BASE FLOW $\times 10$ CASE AT 5000 YEARS

TABLE 6.5

PORTION OF THE AQUIFERS WITH A TEMPERATURE INCREASE
GREATER THAN 15°C, 30°C, 40°C FOR TIME = 5000 YEARS
(i.e., length of affected aquifer/1100 m)

T	15°C	30°C	40°C
<u>First Series</u>			
Two Aquifers, Vantage Sandstone			
No Flow	1.12	0.88	0.50
Base Flow	1.27	0.94	0.60
Base Flow x 10	2	1.55	1.0
<u>Second Series</u>			
Three Aquifers, Lower Flow Top			
No Flow	1.25	1.08	0.96
Base Flow	1.42	1.19	1.08
Base Flow x 10	3.35	2.39	1.59

5000 years. These numbers have been normalized relative to the half-width of the repository. This table indicates that the base flow is little different from the no flow case and that even for the base flow times ten, the temperature disturbance is limited to 2.0 times the length of the repository. This limited lateral influence on aquifer temperatures should not present significant problems; however it must be noted that the thermal loading (25 W/m^2) results in temperatures in the aquifers that are possibly too high.

The results for the second series of analysis are shown in Figures 6.21, 6.22 and 6.23, where the temperature distribution after 5000 years is shown for the three flow conditions. The hypothetical lower aquifer was modelled as a zone 4 m thick with hydraulic properties the same as assumed for the Vantage Sandstone. However, because it is within 60 m of the repository level, it has a more significant impact on the temperature distribution than the other two aquifers modelled above. Table 6.5 lists the length of lower aquifer in which the temperature change exceeds 15° , 30° and 40°C .

The above analysis models an extremely simplified geology and mechanism of heat transfer. No account was taken in this analysis of how the temperature changes will influence the groundwater flow regime. This factor is considered in the next section. The geology of the repository site is unclear at this time so the continuity and frequency of possible aquifers are unknown.

TEMPERATURE CONTOURS FOR TIME= 5000. YEARS

Horizontal and Vertical Scales Are Equal

FIGURE 6.21

TEMPERATURE CONTOURS (DEGREES CENTIGRADE) AFTER 5000 YEARS FOR THE NO FLOW CASE

TEMPERATURE CONTOURS FOR TIME= 5000. YEARS

Horizontal and Vertical Scales are Equal

FIGURE 6.22

TEMPERATURE CONTOURS (DEGREES CENTIGRADE) AFTER 5000 YEARS FOR THE BASE FLOW (1×10^{-7} METERS PER SECOND) CASE

TEMPERATURE CONTOURS FOR TIME= 5000. YEARS

Horizontal and Vertical Scales are Equal

FIGURE 6.23

TEMPERATURE CONTOURS (DEGREES CENTIGRADE) AFTER 5000 YEARS FOR THE BASE FLOW $\times 10$ (1×10^{-6} METERS PER SECOND) CASE

7.0 GROUNDWATER FLOW AND THERMO-MECHANICAL RESPONSE

7.1 Hydrology

7.1.1 Introduction

The hydrology of the Pasco Basin is being extensively studied by Rockwell. In this section, only a brief overview of the Pasco Basin hydrology is included. The hydrology has been divided into four distinct zones: the unsaturated zone above the water table in the unconsolidated sediment; the unconfined aquifer in the unconsolidated sediment; the uppermost confined aquifers contained in the Mabton and Quincy interbeds; and the Grande Ronde Basalt. The Columbia River Basalt in the Pasco Basin consists of lava flows which were produced by repeated eruptions in the Miocene time. These basalts extend to depths in excess of 1500 meters and represent an accumulation of continental basalt. Within the basalt, sedimentary deposits, called interbeds, were often formed between flow periods when lakes or streams developed on top of the basalt flows. The rock structure is dominated by the horizontal layering of flows and interbeds, but some folding and faulting are present.

A generalized cross section trending approximately north-south through the Pasco Basin is illustrated in Figure 7.1. This cross section through the Hanford Site shows the surface topography, unconsolidated sediments overlying the basalt, several basalt flows, and significant interflows. This figure does not indicate the large number of basalt flows that are present, varying in thickness from meters to hundreds of meters. A typical flow can be divided into three major zones: a weathered top, which is often relatively fractured and porous; the entablature, which is composed of an irregular joint pattern, sometimes resembling slender

FIGURE 7.1

**GENERALIZED CROSS SECTION APPROXIMATELY NORTH-SOUTH
THROUGH THE PASCO BASIN**

curved columns; and the colonnade at the bottom of the flow. The colonnade contains a regular pattern of vertical joints which form long, hexagonal columns. The flow tops can have different mechanical and hydrological characteristics than the denser basalts found in the colonnade and entablature. The interbeds are sedimentary deposits consisting of sandstone, clays, diatomaceous or tuffaceous materials. Characterizing the thermo-mechanical and hydrological properties of the interbeds is difficult at present, because of the great range of materials, porosity, degree of consolidation, etc., that exist.

7.12 Hydraulic Properties

Intact Basalt

La Sala and Doty (1971) report the results of laboratory permeability tests performed on intact basalt specimens taken from the core of drill hole DC-1, which is located on the Hanford Site. These tests were performed in conjunction with a field testing program completed in the same drill hole. The results are shown in Table 7.1.

TABLE 7.1
LABORATORY PERMEABILITY RESULTS FOR BASALT
(After LaSala and Doty, 1971)

CORE NUMBER	DEPTH (ft.)*	PERMEABILITY (m/sec)	POROSITY (%)	REMARKS
6	2381.4 - 2384.6	1.3×10^{-10}	9.8	Mod. vesicular
7	2779.0 - 2779.8	2.1×10^{-10}	10.5	-
8	2946.8 - 2950.1	1.1×10^{-10}	25.4	Very vesicular
13	3127.1 - 3128.0	6.7×10^{-11}	2.1	Dense
28	4285.0 - 4285.5	1.4×10^{-10}	10.9	Mod. vesicular

*Units from core log.

These laboratory results reveal that intact basalt has very little ability to transmit water through intergranular pore spaces, even in the case of very vesicular top flows (i.e. the vesicles are not interconnected). La Sala and Doty conclude that the basalt rock mass derives its permeability mainly from fractures. The hydraulic conductivity of the rock mass is discussed in the next section.

The porosity of the intact basalt varies significantly depending upon the location within the flow. For top flows the porosity can be higher than 25% (see Table 7.1) whereas the dense basalts are often lower than 1% (see Agapito et al. 1977.) From a hydrological sense the apparent or interconnected porosity (effective porosity) is important and because of the vesicular nature of the basalt pore spaces the effective porosity can be significantly less than the total porosity. The test results presented by Duvall et al. 1978 for the Pomona flow indicate apparent porosities less than 3% .

Basalt Rock Mass

The permeability of the basalt rock mass can be entirely attributed to the presence of fractures in the intact basalt, since even the highly vesicular but intact flow tops have a low intergranular permeability. Thus, characterizing the hydraulic properties of the rock mass consists of identifying the fracture zones and measuring their hydraulic properties.

Definition of the groundwater conditions beneath the Hanford Site has been the subject of many studies since the 1940's by the U. S. Geological Survey (see Newcomb, et al., 1972). Deju, et al., 1977 summarize these studies. LaSala and Doty (1971) report the results of a series of injection, swabbing, and pumping tests performed on test intervals in drill hole DC-1,

which is located near the center of the Hanford Site. Many of the test intervals include both fracture zones and sedimentary interbeds, and a large number of lithologic units were untested. However, La Sala and Doty estimated the permeability of other units by assuming a correlation between the geophysical log and hydraulic properties. Their results for typical examples of each lithologic unit are given in Table 7.2.

TABLE 7.2

PERMEABILITY VALUES FOR TYPICAL LITHOLOGIC UNITS IN DRILL HOLE DC-1
(After LaSala and Doty, 1971)

DESCRIPTION	PERMEABILITY (m/sec)	ESTIMATED EFFECTIVE POROSITY
Dense basalt above 300 m	1×10^{-7}	1%
Dense basalt below 300 m	1×10^{-8} to 5×10^{-9}	1%
Vesicular basalt	3×10^{-8} to $- \times 10^{-9}$	5%
Fractured or weathered basalt	2.4×10^{-5} to 1×10^{-7}	10%

These results reveal that even the most impermeable in situ basalt has a permeability one to four orders of magnitude greater than the laboratory specimens.

Interbeds

As many as nine significant sedimentary interbeds have been identified in the Upper and Middle Yakima basalt sequence. Outcrops and core logs of boreholes in the Pasco Basin reveal that these interbeds are generally fine-grained sandy, clayey, tuffaceous, or diatomaceous rocks, with a number of these different rock types often occurring within a single interbed. Conglomerates with gravel or pebble to cobble-sized basaltic eject in a fine-grained matrix also occur.

The thickness and areal extent of the inhomogeneities, as well as their mechanical, thermal, and hydraulic properties will determine the effect they have on the overall properties of the basalt sequence. Laboratory test data are unavailable for the interbed rocks of the Pasco Basin; however, the hydraulic properties of the interbed rocks in situ are given by La Sala and Doty (1971).

The interbed materials offer variable hydrologic characteristics. Some of the coarse sandstone interbeds are potential aquifers, but those with significant clay factors are relatively impermeable. Newcomb, et al. 1972 summarize the relative hydraulic characteristics of the interbeds as "overall, these sedimentary layers within the top part of the basalt have yielded less water to wells than the more permeable stratigraphic zones of the basalt." La Sala and Doty (1971) characterize the hydraulic conductivity of sand interbed material as 10^{-5} m/sec. which is about half of their estimate of the conductivity of the fractured or weathered interflow basalt. They estimate the effective porosity to be 20%.

7.1.3 Simplified Stratigraphic Section

In this report a simplified stratigraphic section of the Pasco Basin was used as input for the coupled thermal, fluid and stress analysis. It was considered more worthwhile at this stage of the investigations to analyze simple geologic configurations in order to aid insight into the groundwater flow behavior. As knowledge accumulates on the hydrologic properties, areal extent, etc. of the materials in the basin the stratigraphic unit will be updated and modified accordingly. The simplified section analyzed in this report is illustrated in Figure 7.2. The section consists of an upper unconsolidated sedimentary zone, and a homogeneous basalt rock mass except for

FIGURE 7.2

SIMPLIFIED STRATIGRAPHIC SECTION USED IN
COUPLED THERMAL, FLUID AND STRESS ANALYSIS

two permeable layers contained within it, the Vantage Sandstone at 700-m depth and a potentially somewhat fractured basalt at 1182-m depth. The hydrologic properties of the members of this stratigraphic section are listed in Table 7.3.

TABLE 7.3

SIMPLIFIED STRATIGRAPHIC UNIT INCLUDING ASSUMED VALUES

Depth (m)	Description	Permeability (m/sec)	Effective Porosity	
			Case I	Case II
0 to 300	Sediments	1×10^{-6}	0.10	0.10
300 to 700	Moderate to dense basalt	1×10^{-9}	5×10^{-4}	2.5×10^{-3}
700 (4m thick)	Vantage Sandstone	1×10^{-6}	0.10	0.10
700 to 1182	Moderate to dense basalt	1×10^{-9}	5×10^{-4}	2.5×10^{-3}
1182 (4m thick)	Fractured basalt	1×10^{-6}	0.10	0.10
1182 to 3000	Moderate to dense basalt	1×10^{-9}	5×10^{-4}	2.5×10^{-3}

This section was analyzed for two cases I and II, which differ only in the effective porosity of moderate to dense basalts. For Case I an effective porosity of 5×10^{-4} was used for the moderate to dense basalt; while in Case II a value of five times this, that is 2.5×10^{-3} was input. It should be pointed out that both of these values are much lower than the basalt rock mass porosities quoted in Section 7.1.2. By using these lower values the transport times of particles moving through the basalt will be 20 and 4 times faster for effective porosities of 5×10^{-4} and 2.5×10^{-3} respectively compared with an effective porosity of 1%.

7.2 Coupled Thermal and Fluid Flow

7.2.1 Numerical Procedure

A description of the numerical procedure used here is given in Appendix 5, along with checks on program accuracy. In its present form it is a two-dimensional model with the solution to the governing mathematical equations being determined by an alternating-direction-implicit technique with integrated finite differences. The resulting algorithm is numerically stable and possesses an accuracy of the second-order in the space domain and of the first-order in the time domain. The program is suitable for solving both steady- and unsteady-state flow and takes into account temperature-dependent water properties. The program has been written with extensive plotting routines for constructing plots of darcy velocities, temperatures, particle velocities, streamlines and particle tracking routines. The particle tracking routines record tracks made by a particle as it moves through the problem domain. The tracking routines have been tested for accuracy by simple examples and extensive tests are being undertaken to ensure accuracy of the solution procedure.

7.2.2 Input Data

The hydrological properties of the members of the simplified stratified stratigraphic section as shown in Figure 7.2 have been quoted in Table 7.3. The problem domain was 20 kilometers horizontally and 3 kilometers in depth. The hydrological boundary conditions consisted of an impermeable bottom, regional flow from left to right of gradient 1.5 meters per kilometer, and a free upper surface. The geothermal gradient was assumed to be 20°C at the surface with a gradient of 0.04°C per meter depth. The repository was modelled by 2-dimensional plane geometry with a horizontal

dimension of 3000 meters and a gross plan areal thermal loading of 25W/m^2 . The power decay curve of the 10-year-old waste was represented by a six component exponentially decaying heat source. The source strength is described by Equation 5.1 and the coefficients of this equation Q and λ are given in Table 7.4. Mesh details are shown in Figure 7.3.

TABLE 7.4

SIX-COMPONENT EXPONENTIALLY DECAYING HEAT SOURCE

Component	Q/Q_0	Half-Life (years)	λ (years ⁻¹)
1	0.00756	30140	2.3×10^{-5}
2	0.0151	6970	9.945×10^{-5}
3	0.1404	396	1.75×10^{-3}
4	0.677	32	2.167×10^{-2}
5	0.0544	17.2	4.03×10^{-2}
6	0.1093	2.38	2.912×10^{-1}

The thermal and mechanical properties of the members of the stratigraphic sections are as listed in Table 7.5.

TABLE 7.5

THERMAL-MECHANICAL PROPERTIES OF STRATIGRAPHY UNITS

Member	Unconsolidated Sediments	Sandstone	Moderate to Dense Basalt
Young's Modulus (MPa)	1×10^3	5×10^3	5×10^4
Poisson's Ratio	0.4	0.2	0.2
Coeff. of Linear Thermal Expansion (°K ⁻¹)	5.0×10^{-6}	10×10^{-6}	5.4×10^{-6}
Heat Capacity (J/m ³ °K)	2.2×10^6	1.5×10^6	3×10^6
Conductivity (W/m °K)	1.95	4.2	1.95

FIGURE 7.3

FINITE DIFFERENCE AND FINITE ELEMENT MESH GRID FOR
SIMPLIFIED STRATIGRAPHIC SECTION

The in situ stress field was assumed to be lithostatic with the vertical stress equivalent to the overburden pressure.

7.2.3 Thermal and Fluid Flow Analysis

The coupled thermal and fluid flow analyses were undertaken on two cases I and II; only the effective porosity of the moderate to dense basalt was changed in the two cases, the effective porosity of the moderate to dense basalt was increased. Only a portion of the results will be presented in this section and the remainder have been placed in Appendix 6 for the benefit of clarity.

The particle tracks for particles released after an elapsed time of 100 years for Case I are illustrated in Figure 7.4. Five particles were released and their history was recorded for the entire duration of the runs (in this case 10,000 years) or until the particle encountered a boundary of the problem domain. The numbers marked on the tracks are the number of years in thousands, from time zero for the particle to reach that particular point. It should be pointed out that this figure is scaled approximately 7 to 1 horizontally to vertically and significantly distorts moderate curves into abrupt changes.

The influence of the upward buoyancy force resulting from the heating of the groundwater and the development of natural convective cells can be seen from the trace of the particle paths. The particle released at the far right of the repository entered a downward convective cell before it reached the Vantage Sandstone (depth of 700m). This particle did eventually rise at approximately 2,500 years and then entered another downward convective cell at 5000 years. The particle released second from the right entered the Vantage at approximately 1000 years then travelled along the Vantage for 750 meters then rose to almost the level of the unconsolidated sediments, and entered a downward current to finish 500 meters below the repository at 10,000 years. The remaining three particles all rose to the Vantage,

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 500 YEARS

FIGURE 7.4

PARTICLE TRACKS FOR CASE I - PARTICLES RELEASED AT 500 YEARS

travelled horizontally along it, then rose to the bottom of the unconsolidated sediments. At this level they proceeded to travel horizontally at a depth of approximately 300 m, to finish at 10,000 years almost 5 kms horizontally from their initial released positions.

The temperature distribution around the repository at an elapsed time of 500 years is illustrated in Figure 7.5. The Darcy and particle flow velocities within the problem domain are shown as vectors in Figures 7.6 and 7.7, respectively. The upward motion of the fluid particles up through the repository region are clearly illustrated in Figure 7.7.

The tracks of five particles released at repository level after an elapsed time of 5000 years for Case I are illustrated in Figure 7.8. Except for the particle released from the far right of the repository, all particles again moved vertically away from the repository up to the Vantage Sandstone, then travelled a short horizontal distance within the Vantage Sandstone and then rose to the bottom of the unconsolidated sediments. From here, the particles moved approximately 3000 meters horizontally 5000 years after the time of their release. The particle released from the far right of the repository, initially rose vertically to the Vantage Sandstone and travelled a short distance horizontally within the Vantage Sandstone. It then entered a downward convective cell, travelled downward to approximately 1500 meters depth, then rose vertically to the unconsolidated sediments. The temperature contours and approximate stream lines for an elapsed time of 5000 years are illustrated in Figures 7.9 and 7.10, respectively. The convective cell on the downstream side of the repository is present as was the case for an elapsed time of 500 years. The Darcy and particle velocities are plotted as vectors for this case in Figures 7.10 and 7.11, respectively.

HANFORD HLW REPOSITORY 25W/M2

TEMPERATURE PLOT

TIME = 500 YEARS

FIGURE 7.5

TEMPERATURE CONTOURS AT ELAPSED TIME OF 500 YEARS

HANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 500 YEARS

FIGURE 7.6

DARCY FLOW VELOCITIES AT ELAPSED TIME OF 500 YEARS

HANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 500 YEARS

FIGURE 7.7

PARTICLE FLOW VELOCITIES FOR CASE I AT 500 YEARS

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 5000 YEARS
DISTANCE (km)

FIGURE 7.8

PARTICLE TRACKS FOR CASE I - PARTICLES
RELEASED AT 5000 YEARS

HANFORD HLW REPOSITORY 25W/M²

TEMPERATURE PLOT

TIME = 5000. YEARS

FIGURE 7.9

TEMPERATURE CONTOURS AROUND REPOSITORY AT 5000 YEARS

HANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 5000 YEARS

FIGURE 7.10

DARCY FLOW VELOCITIES AT ELAPSED TIME OF 5000 YEARS

HANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 5000 YEARS

FIGURE 7.11

PARTICLE FLOW VELOCITIES FOR CASE I-AT 5000 YEARS

The particle tracks of fluid particles released at elapsed times of 500 and 5000 years for Case II are illustrated in Figures 7.12 and 7.13. The two Cases I and II only differ in the values of the effective porosity of the moderate to dense basalt. In Case II the moderate to dense basalt had an effective porosity five (5) times that for Case I. This difference results in particles moving through the moderate to dense basalt at much slower velocities in Case II compared to Case I. The particles released at an elapsed time of 500 years, Figure 7.13, initially all move vertically. All except the right-hand-released particle rise to the Vantage Sandstone travel horizontally along it for a short distance then rise to the unconsolidated sediments. The three leftmost particles upon reaching the unconsolidated material travel approximately 9 kms horizontally within 20,000 years. The second particle released from the right reaches the sediments, travels approximately 2 kms horizontally at a depth of 300 m then upon reaching a downward convective cell proceeds downwards and finishes at an elapsed time of 20,000 years at the repository level. The particle released from the right of the repository completes a full elliptical path then rises vertically to the upper sediments and finally enters a downward convective cell to finish at a depth of 400 m after 20,000 years elapsed time. The particles for Case II released at 5000 years, Figure 7.13, follow similar paths to those particles released at 500 years.

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 500. YEARS
DISTANCE (km)

FIGURE 7.12

PARTICLE TRACKS FOR CASE II - PARTICLES RELEASED AT 500 YEARS

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HANFORD HLW REPOSITORY

RHO-BWI-C-23
25W/M2

TRACKS OF PARTICLES RELEASED AT 5000 YEARS
DISTANCE (km)

FIGURE 7.13

PARTICLE TRACKS FOR CASE II - PARTICLES RELEASED AT 5000 YEARS

7.3 Coupled Stress, Thermal and Fluid Flow

7.3.1 Program Coupling

The coupled thermal and fluid flow analyses were undertaken by the finite difference program GWTHERM. The extension of this coupling to include the effects of stress and deformation on heat and mass transfer was undertaken indirectly by separate programs. For example, the heat and mass transfer calculations were undertaken for a number of time steps, then the stress and deformations due to changes in the temperature field were computed by a finite element program DAMSWEL (Dames & Moore Swansea Finite Element program). The changes in stress and deformation modify the hydraulic properties of the material, then these new hydraulic properties are input into GWTHERM for continuation of the calculation loop. This loop is illustrated diagrammatically in Figure 7.14. The stress calculations were not linear elastic, but incorporated a no-tension non-linear compression failure criterion with temperature-dependent material properties. The validity of this coupling, that is the estimation of the loop time step increment which does not affect the results, can only be determined by running a problem at different step increments.

The programs GWTHERM and DAMSWEL both used similar grids and mesh for the discretization of the problem domain. The finite element mesh consisted of eight noded isoparametric quadrilaterals with the temperature computed at the Gauss points by linear interpolation from the finite difference grid. The setting up of the load vector for DAMSWEL was undertaken by a separate special purpose program called LOAD, as indicated in Figure 7.14. The reason for analyzing this problem by a number of separate programs was to provide an easy means of local file manipulation with restarting and stopping capabilities.

FIGURE 7.14

COUPLED STRESS-THERMAL AND FLUID FLOW ANALYSIS LOOP

7.3.2 Experimental Studies

The study of flow through fissures has been based primarily on the application of classical hydrodynamic theories relating to incompressible viscous flow between parallel plates. The majority of studies have assumed a Darcy type of flow law:

$$v = k_f i \quad 7.1$$

where v is the velocity, k_f the hydraulic conductivity of a fracture and i is the hydraulic gradient.

If it can be assumed that the fracture can be represented by a parallel-plate system, the proportionality constant k_f is given exactly by Lamb (1957).

$$k_f = \frac{ge^2}{12\nu} \quad 7.2$$

where g is the acceleration due to gravity, e the aperture of the fissure and ν the kinematic viscosity of the fluid.

A very limited amount of laboratory data on the permeability of fractures exists. Extensive tests on simulated fractures (Louis, 1969), have been carried out and Figure 7.15 illustrates some of the results from these tests. It is interesting to note from this diagram that the transition from laminar to turbulent flow in a simulated fracture begins earlier than in pipe flow. Iwai (1976) has undertaken a number of experiments on a single fracture in basalt in order to determine the validity of the cubic law between continuum permeability and the fracture aperture, as given in Equation 7.3, for a single set of parallel fissures at a spacing of D :

$$k = \frac{ge^3}{12\nu D} \quad 7.3$$

Plot shows friction factor versus Reynolds number for various fissure apertures and surface roughness

FIGURE 7.15

LARGE-SCALE LABORATORY TESTS ON SIMULATED FRACTURES (after Louis, 1969)

where k is the continuum permeability of the fractures.

Due to the highly non-linear relationship between velocity and hydraulic gradient in a fissure (of order e^2), it is evident that any change in aperture will substantially alter the flow rate. The normal stress-deformation behavior of fractures is not only non-linear, but also exhibits cyclic effects and permanent set. A number of laboratory tests have been performed to study the effect of normal loading on fissure closure. Figure 7.16 demonstrates the above-mentioned effects as far as a fracture in basalt is concerned. This specimen did not exhibit significant cyclic effect, in fact the curves plotted for Runs 1 and 2 are approximately similar. Iwai concluded that Goodman's dimensionless expression for the stress-deformation curve of a fracture was applicable to his results. This curve proposed by Goodman (1976) is illustrated for the idealized case in Figure 7.17. The expression is given by Equation 7.4.

$$V_{mc} \frac{\Delta V}{-\Delta V} = A \left(\frac{\sigma_n}{\xi} \right)^t \quad (\Delta V < V_{mc}) \quad 7.4$$

where V_{mc} , ΔV and ξ are as illustrated in Figure 7.17, σ_n is the normal stress acting and A and t are constants.

Iwai determined the constants A and t for a fracture in a basalt and these computed values for two cycles of loading are given in Table 7.4. In the experiments conducted by Iwai the seating stress, ξ , for the basalt specimen was due only to the weight of the upper rock sample ($\xi = 0.022$ MPa).

TABLE 7.4

THE VALUES OF CONSTANTS A AND t

Rock Type	Number of Run	A	t
Basalt	First	0.0445	0.5
	Second	0.046	0.5

FIGURE 7.16

NORMAL LOADING OF A FRACTURE IN BASALT (IWAI, 1976)

FIGURE 7.17

IDEALIZATION OF NORMAL CLOSURE OF A JOINT (GOODMAN, 1976)

The comparison of the dimensionless deformation versus dimensionless stress for the experimental data of Iwai and Goodman's expression is illustrated in Figure 7.18.

The effect of normal stress on fracture permeability is illustrated in Figure 7.19 for a single fracture in basalt. It is interesting to note the minor changes in fracture permeability in the range of 5 to 20 MPa normal stress. The comparison of the test results by Iwai with the cubic law is illustrated in Figure 7.20 for a fracture in basalt. The agreement appears excellent except in the region of minimum fracture apertures considered. Iwai concluded that the reason for the discrepancy at the lower range of apertures was due to the poor uniformity of the flow at these loads. This fact is illustrated in Figure 7.21.

The change in permeability with normal stress was determined by Iwai for a fracture in basalt. This expression is given by Equation 7.5.

$$\frac{k_d}{k_{d10}} = \frac{1}{1 + A \left(\frac{\sigma_n}{\xi} \right)^{\frac{1}{3}}} \quad 7.5$$

where k_d and k_{d10} are the permeabilities at normal stresses at σ_n and ξ respectively.

The changes in permeability of the basalt media were determined as given by Equation 7.5. The effective (flow) porosity of the media was assumed to be directly related to the fracture aperture. The changes in fracture aperture with normal stress are given by Equation 7.4.

7.3.3 Assumptions

The coupled thermal, fluid and stress analysis were undertaken assuming the expressions given by Equations 7.4 and 7.5 were valid for predictive changes in porosity and permeability of the basalt rock. The basalt rock

FIGURE 7.18

DIMENSIONLESS DEFORMATION VERSUS DIMENSIONLESS
STRESS FOR BASALT SAMPLE (Iwai, 1976)

FIGURE 7.19

PERMEABILITY CHANGES OF A SINGLE FRACTURE IN BASALT
DUE TO NORMAL LOADING (Iwai, 1976)

FIGURE 7.20

COMPARISON OF EXPERIMENTAL RESULTS FOR RADIAL FLOW THROUGH
TENSION FRACTURE IN BASALT WITH CUBIC LAW (Iwai, 1976)

FIGURE 7.21
IRREGULAR OPEN SPACE AROUND THE INJECTION
HOLE OF BASALT SAMPLE (Iwai, 1976)

for these preliminary studies were assumed to contain only horizontal and vertical joint sets.

7.3.4 Thermal, Fluid Flow and Stress Analysis

A complete (thermal, fluid and stress) coupled analysis was undertaken for Case I, previously analyzed solely by GWTHERM (coupled thermal and fluid flow). The hydraulic and thermal properties of the basalt were the same as for Case I as described in Section 7.1. The thermo-mechanical properties of the basalt rock mass were as mentioned in Section 5.0; that is, Young's modulus of 4.8×10^4 MPa, Poisson's ratio of 0.2, coefficient of linear thermal expansion of $5.4 \times 10^{-6}/^\circ\text{C}$ and joint normal closure relationship as described in Section 7.3.1. The coupling between stress and the thermal-fluid analysis was undertaken in an implicit fashion at the following elapsed times 100, 500, 1000 and 5000 years. These time-step increments were chosen after thermal stress analysis had indicated an initial rapid change in thermal stress for elapsed times up to approximately 500 years followed by a period of more gradual change in thermal stress, greater than 500 years. The resulting dependence of the solution on these time-step increments has not been determined at this time, but is currently under investigation.

Thus at zero elapsed time the stratigraphic section with associated hydraulic properties is as shown for Case I, Figure 7.1. At an elapsed time of 100 years the stresses have been modified by the thermal power output of the nuclear waste. The maximum change in stresses from the initial ambient case to an elapsed time of 100 years for a gross areal thermal loading of 25W/m^2 was approximately 25 MPa horizontally in the region of the repository. Increasing the horizontal stresses will result in higher normal stresses on vertical joint sets. For this elapsed time the maximum change in

permeability was a factor of approximately two (2), that is from 1×10^{-9} m/sec. to 5×10^{-10} m/sec.

Rather than re-present large numbers of plots which would be similar to those presented in 7.1 and Appendix 6, only those plots that alter significantly are presented. The particle plots most affected by the coupling of stress and thermal-fluid analyses were for particles released at small elapsed times. The traces of particles released at 100 years are illustrated in Figure 7.22 and for the complete coupled analysis and Figure 7.23 for the coupled thermal fluid analysis. The differences between these two sets of particle tracks are: (a) particle tracks computed by the completely coupled program move more slowly away from the repository initially than do those computed by the thermal and fluid flow analysis; (b) the particle released from the left side of the repository turns downward into a convection cell for the completely coupled case, while for the coupled thermal and fluid analysis this particle moves up to the Vantage Sandstone and then enters a downward convective cell; (c) the particle released from the right-hand side of the repository finished at 10,000 years below and to the left of its original position for the completely coupled case, while for the thermal and fluid flow analysis this particle at 10,000 years is to the right and below its original position.

Due to the limitations of the finite element program to model infinite regions, the resulting thermal stress distribution did have minor perturbations resulting from the imposed boundary conditions. Since the problem domain is a semi-infinite media it is planned in the short term to use the boundary element technique to replace the finite element method in the thermal fluid and stress coupling loop. However, investigations are ongoing to incorporate infinite finite elements into the analysis; this should eliminate

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 100. YEARS

FIGURE 7.22

TRACKS OF PARTICLES RELEASED AT 100 YEARS FOR THE
COUPLED THERMAL FLUID AND STRESS ANALYSIS - CASE I

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 100. YEARS
DISTANCE (km)

FIGURE 7.23

TRACKS OF PARTICLES RELEASED AT 100 YEARS FOR THERMAL
AND FLUID FLOW ANALYSIS - CASE I

these perturbations due to artificially imposed boundary conditions.

The results from this analysis (coupled thermal, fluid and stress) should be considered as a demonstration of capability, rather than as informative results; the reasons being that the results are founded on relationships determined from a limited laboratory testing program on single fissures and several factors such as changes in permeability with depth, effective stress considerations, etc., have not been considered at this stage.

8.0 PRELIMINARY THERMAL LOADING GUIDELINES

8.1 Canister Scale

In the short term (less than one year elapsed time since the canister was placed) the temperatures around the base case canister are moderate (see Chapter 4.0). With time the interaction between neighboring canisters occurs and gives rise to increased temperatures. This effect of canisters interacting with its neighbors is illustrated diagrammatically in Figure 8.1. For a canister 5m long with an initial thermal output of 1 kW the temperature time history is similar to that shown by the full line in Figure 8.1. This curve has an initial peak at approximately 1 year and then peaks again due to the interaction of the neighboring canisters. From a maximum temperature limit criterion, it would be sensible to ensure that the initial peak is similar to the later one. This point is illustrated by the dashed line. The consequences of following this dashed line will give rise to the following changes to the base case; namely: (a) allowable increase of thermal energy per canister, approximately 2 to 2.5 kW for a 5m length; and (b) increased spacing between canisters. This will result in a reduction of the number of canisters and boreholes required compared to the base case for the same thermal energy output of the waste.

The stresses in the basalt during the initial temperature peak of the base case are moderate and are well below the 135 MPa (20,000 psi) considered here to be a satisfactory working level of stress around the canister boreholes. This figure of 135 MPa is purely a preliminary estimate and should only be considered for the parametric analysis and assessment. The level of allowable working stress around the canister borehole will be updated when data are available from proposed laboratory and field trials.

At elapsed times greater than one year thermal interaction between the

FIGURE 8.1

DIAGRAMMATIC SKETCH OF ROCK/CANISTER TEMPERATURE HISTORY

canisters is present. Thus by the time 5 and 25 years have elapsed moderate increases in temperature have occurred accompanied by significant increases in stresses. The rock stresses around the canister boreholes are now dominant and for the base case at 5 years elapsed time, the rock stresses are approximately the same as the proposed working level.

8.2 Room Scale

The temperatures around the room at elapsed times of 5 and 25 years are significant but do not give rise to concern, except for possibly human comfort, ventilation, etc.; the stresses on the other hand especially in the floor control the thermal energy input to a room. The allowable working level of stress for the basalt around the rooms was preliminary and taken to be 67 MPa (10,000 psi). As stated in Section 8.1 the working levels of stress assumed for this parametric study are only preliminary and will be updated when more data are available. At an elapsed time of 5 years the floor stresses control the thermal energy loading per room but do not control the areal thermal loading because of minor thermal interaction between rooms. From the preliminary working stress level around the rooms an areal thermal loading of 75 W/m^2 is satisfactory; however, there exist significantly high stresses around the canister boreholes which could result in borehole wall failure. To avoid exceeding the borehole wall stress level after 5 years, the areal thermal loading of 75 W/m^2 will need to be reduced to approximately 25 W/m^2 . However since no three-dimensional thermo-mechanical analyses have been undertaken at this time this value is purely a preliminary estimate.

At an elapsed time of 25 years, the stresses in the floor of the rooms control the thermal energy loading per room and the gross areal thermal loading. This is due to the significant thermal-mechanical interaction between neighboring rooms. To avoid exceeding the preliminary working stress level around the rooms a gross areal thermal loading for the base case of 25 W/m^2 is satisfactory. However, as found in the case of 5 years elapsed time, the working stress around the canister borehole will be exceeded. To avoid over-stressing of the canister borehole walls the areal thermal loading for an elapsed time of 25 years will need to be reduced to approximately 20 W/m^2 . As stated earlier until three-dimensional analyses have been undertaken these estimates must be considered preliminary.

For a retrievability period of 50 years the allowable thermal loadings are much the same as for the 25-year case. However, even though the stresses and temperatures do not increase over the longer retrievability period, additional deterioration of the rooms will result from time-dependent movements.

The parametric study indicates that the base case canister layout and room shape is not optimal. Multiple rows of canisters in the floor and walls result in more even thermal loading and could result in higher initial thermal loadings. Similarly arched or circular rooms could improve room stability. More definite recommendations on canister location room shape and room spacing will follow a study on design criteria now under way.

8.3 Regional Scale

The thermal output from the nuclear wastes give rise to ground temperature increases and modifications to the groundwater flow regime. Analyses have been undertaken at a gross thermal loading of 25 W/m^2 . The resulting increases in temperatures and buoyancy forces significantly modify the

regional groundwater flow. Immediately above the repository, in the impermeable, low-porosity basalts, the flow is vertical. Within interbeds or top flows, which are relatively permeable and porous, the flow is horizontal. Eventually the groundwater which has passed through the repository reaches the unconsolidated sediments above the basalt and flows horizontally near the sediment/basalt contact. No groundwater particles that passed through the repository reached the biosphere in any of the analyses performed (all runs were for at least 10,000 years).

The coupled stress, heat and groundwater flow analysis indicated a change in permeability near the repository of a factor of two (2), but tended to slow down the groundwater flow.

The above analyses were made on simplified geological sections assuming such things as total shaft and repository sealing, resaturation of the repository, limited number of highly permeable and porous horizontal interbeds or top flow, a slight regional groundwater cross flow and isotropically permeable basalt. Any conclusions drawn from the analyses at this time would be premature; however, it appears that a gross thermal loading of 25 W/m^2 could be acceptable on a regional scale.

9.0 OTHER FACTORS INFLUENCING REPOSITORY PERFORMANCE

The foregoing parametric study has included many of the important parameters that will control or influence the final repository design. However, there are many design layout and operational factors that could have an overriding influence on such things as allowable power per canister, loading per room and gross thermal loading; hence, no firm recommendations on basic design parameters can be given until these additional factors are evaluated. We have listed some of them below that will influence the thermo-mechanical response and hence could dictate lower or higher waste emplacement densities. These factors were not explicitly covered in the above parameter study although some have been included in part.

1. Geology. Local geological features such as joint infilling materials, inclusions, and variations in basalt properties, could have a major influence on canister lining requirements etc.
2. Regional geology. Influence of interbeds on groundwater flows, stability of rooms and shafts, impact of faults or zones of reduced rock quality on the above.
3. Seismicity. Impact of ground vibrations from distant earthquakes or potential earthquakes within the repository site.
4. Moisture changes within the basalt and joint material could cause changes in thermal properties and shrinkage. This could impact canister design, borehole stability, and room stability.
5. Waste form and packaging. Some study of the impact of various forms of waste was included in the parameter study but other packaging concepts different shafts, reprocessing and age of waste could be important.
6. Retrievability period and concept could influence borehole configuration and allowable safety factors.

7. Borehole linings could allow high stresses; hence, higher thermal inputs.
8. Room support. Lining, bolting will influence room stability during period of retrievability.
9. Backfilling form and sequence must be examined closely to determine impact on regional stability and allowable loadings.
10. Handling facilities. Remote handling facilities could require increased room stability, lower probability of roof falls etc.
11. Ventilation, heat removal. Schemes to remove heat from the canister or rooms over long periods of time could drastically alter repository layouts.
12. Microbiology changes resulting from temperature changes in the groundwater may be important and result in lower allowable gross thermal loads than anticipated.
13. Site specific groundwater conditions and repository location, such as above or below the groundwater, obviously will impact the final repository
14. Economic considerations. If policy is to demonstrate concept, with no concern for optimizing cost thermal loadings can be dropped and repository performance confidently predicted for large time spans.

Some of the above considerations are outside of the scope of a thermo-mechanical, rock mechanics analysis, but many will impact the allowable stresses, temperatures or groundwater flow that are of direct concern.

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APPENDIX 1

A MATHEMATICAL MODEL FOR TRANSIENT HEAT CONDUCTION

APPENDIX 1

A MATHEMATICAL MODEL FOR TRANSIENT HEAT CONDUCTION

1.0 INTRODUCTION

The primary purpose of this appendix is to present HEAT, a Lagrangian finite difference code capable of predicting heat conduction in an orthotropic conducting medium.

The following energy conservation equation, the heat conduction equation, is solved by HEAT:

$$\dot{E} = \nabla \cdot \vec{k} \nabla T + P \quad (1-1)$$

where E is the internal energy per unit volume, T is the temperature, k is the thermal conductivity, and P is the source power density. The finite difference equations used to approximate this differential equation are those developed by Wilkins (1964). The numerical formulation is almost identical to that used in PISCES 2DL (see Jardin, et al., 1972).

A detailed description and analysis of the finite difference equations in HEAT which approximate Equation 1-1 follow. In addition, the results of several HEAT calculations are presented and compared to the analytical solutions of the heat conduction equation.

2.0 FINITE DIFFERENCE EQUATIONS

The differential equations that govern the conduction of heat in a continuum are approximated by difference equations applied to a network of zones that describe the physical space occupied by the conducting medium (see Figure 1). The Lagrangian formulation of the difference equations requires that each zone contain a constant mass. The temperature gradients are calculated at zone corners (grid points) defining zonal boundaries, while temperature and internal energy are defined as averages over zonal interiors. At each time step, incremental changes in internal energy are computed for each zone from the temperature gradients of the four surrounding grid points. When energy increments have been calculated for all zones, the complete mesh is scanned in order to update the temperature

GOVERNING EQUATIONS: $\dot{E} = \nabla \cdot K \nabla \vec{T} + P$

BOUNDARY CONDITIONS: $T = T_i = 0$ ON S_1

$$\frac{\partial T}{\partial \vec{n}} = 0 \text{ ON } S_2$$

FIGURE 1

EQUATIONS, SOLUTION DOMAIN AND DISCRETIZATION

of the zones. The whole cycle described above then repeats for the next time step.

It is important to realize that in the explicit formulation the energy of each zone is "frozen" for one time step, since the time step is taken so small that information is unable to physically propagate to the next zone. This means that each zone is independent for that time period: the temperature calculated is unique for that zone and is not influenced by what is going on in other zones.

2.1 Basic Equations

For an elemental mass within the conducting medium, conditions of continuity require that during a time interval Δt the quantity of heat flowing in, less the quantity flowing out, plus the amount generated internally by any sources, equals the amount of energy stored within the zone.

$$\dot{E} = \vec{V} \cdot \vec{K} \vec{\nabla} T + P \quad (2.1-1)$$

At each time step, incremental changes in the energy are computed from the temperature gradients and from the heat output of the source as described in Sections 2.1.1 to 2.1.3.

Then, the zone temperatures are updated from the changes in energy. Assuming constant density ρ , constant specific heat C_v and negligible compression energy, the temperature increment is given by

$$\Delta T = \Delta E / \rho C_v \quad (2.1-2)$$

At present, program HEAT is restricted to materials for which Equation 2.1-2 is applicable.

The analysis of transient heat conduction problems involves the solution of Equation 2.1-1 subject to a temperature-energy constitutive relationship such as Equation 2.1-2. In addition, the solution to a particular problem must satisfy the given boundary conditions. Treatment of fixed temperature boundaries is shown in Figures 2 and 3

$$T = T_1 \text{ on } S_1, \quad (2.1-3)$$

and non-conducting boundaries

$$\frac{\partial T}{\partial \hat{n}} = 0 \text{ on } S_2 \quad (2.1-4)$$

is discussed in Section 2.2.

FIGURE 2

INTEGRAL DEFINITION OF GRADIENTS

FIGURE 3

GRADIENTS AT NODES

2.1.1 Gradients

The following integral definitions of partial derivatives are used for the temperature gradients

$$\frac{\partial T}{\partial x} = \int_C T(\hat{n} \cdot \hat{i}) ds \bigg/ \lim_{A \rightarrow 0} A \quad (2.1-5)$$

$$\frac{\partial T}{\partial y} = \int_C T(\hat{n} \cdot \hat{j}) ds \bigg/ \lim_{A \rightarrow 0} A \quad (2.1-6)$$

where C is the boundary of A , s is the arc length, $\hat{n}$ is the unit vector normal to the surface, and $\hat{i}$ and $\hat{j}$ are the unit vectors along the x and y axes, respectively (see Figure 2). In terms of the four zones surrounding a node, the above definitions yield the following expressions for the gradients at that node (see Figure 3):

$$\left(\frac{\partial T}{\partial x} \right)_{i,j} = \frac{1}{A_{i,j}} \left[T_a (y_2 - y_1) + T_b (y_3 - y_2) + T_c (y_4 - y_3) + T_d (y_1 - y_4) \right] \quad (2.1-7)$$

$$\left(\frac{\partial T}{\partial y} \right)_{i,j} = - \frac{1}{A_{i,j}} \left[T_a (x_2 - x_1) + T_b (x_3 - x_2) + T_c (x_4 - x_3) + T_d (x_1 - x_4) \right] \quad (2.1-8)$$

where

$$A_{i,j} = .5 (A_a + A_b + A_c + A_d) \quad (2.1-9)$$

2.1.2 Flux Rate

The heat flux rate, $\dot{Q}$, for each face separating one zone from another is calculated as follows (see Figure 4). The flux rate appropriate to face ab is given by:

$$\dot{Q}_{ab} = \int_{ab} K_{ab} \nabla T \cdot d\vec{A} \quad (2.1-10)$$

FIGURE 4

FLUX RATE ACROSS AN INTER-ZONAL FACE

where K_{ab} is the thermal conductivity of face ab. For systems with planer symmetry (2.1-10), may be approximated by the following formula:

$$\begin{aligned} \dot{Q}_{ab} = & K_{ab_x} \left[.5 \left\{ \left(\frac{\partial T}{\partial x} \right)_1 + \left(\frac{\partial T}{\partial x} \right)_2 \right\} (y_2 - y_1) \right] \\ & - K_{ab_y} \left[.5 \left\{ \left(\frac{\partial T}{\partial y} \right)_1 + \left(\frac{\partial T}{\partial y} \right)_2 \right\} (x_2 - x_1) \right] \end{aligned} \quad (2.1-11)$$

where K_{ab_x} and K_{ab_y} are the average x and y directed thermal conductivities appropriate to face ab, defined by

$$K_{ab_i} = \frac{A_a + A_b}{\frac{A_a}{K_{a_i}} + \frac{A_b}{K_{b_i}}}, \text{ where } i = x \text{ or } i = y \quad (2.1-12)$$

And, for systems with rotational symmetry about the x-axis (2.1-10) may be approximated by:

$$Q_{ab} = \frac{2}{3} \pi K_{ab_x} \left[(y_1 + .5y_2) \left(\frac{\partial T}{\partial x} \right)_1 + (y_2 + .5y_1) \left(\frac{\partial T}{\partial x} \right)_2 \right] (y_2 - y_1) \quad (2.1-13)$$

$$- \frac{2}{3} \pi K_{ab_y} \left[(y_1 + .5y_2) \left(\frac{\partial T}{\partial y} \right)_1 + (y_2 + .5y_1) \left(\frac{\partial T}{\partial y} \right)_2 \right] (x_2 - x_1)$$

The net heat flux into a zone can then be written as the sum of the heat fluxes across the four faces surrounding it (see Figure 5).

$$\dot{Q} = (\dot{Q}_1 + \dot{Q}_2 + \dot{Q}_3 + \dot{Q}_4) \quad (2.1-14)$$

FIGURE 5

FLUX RATE FOR A ZONE

2.1.3 Internal Energy

The increase in the zone's internal energy density due to heat conducted over one time step is computed as the sum of the heat conducted over each of the zone's four faces divided by V , the zone's volume (see Figure 5).

$$E^{n+1} = E^n + \frac{\dot{Q}_1 + \dot{Q}_2 + \dot{Q}_3 + \dot{Q}_4}{V} \cdot \Delta t \quad (2.1-15)$$

If a source is present in the zone, then the energy is given by

$$E^{n+1} = E^n + \frac{\dot{Q}_1 + \dot{Q}_2 + \dot{Q}_3 + \dot{Q}_4}{V} \Delta t + P \Delta t, \quad (2.1-16)$$

where P is the power density of the source at the current point in time.

2.2 Treatment of Boundaries

The thermal boundaries may be non-conducting or fixed temperature boundaries.

(1) Non-conducting boundaries

(a) Non-corner point (see Figure 6).

The components of the gradient are initially defined at P as

$$\left(\frac{\partial T}{\partial x}\right)_P^0 = \frac{1}{A_P} \left[T_a (y_2 - y_1) + T_b (y_1 - y_3) \right] \quad (2.2-1)$$

$$\left(\frac{\partial T}{\partial y}\right)_P^0 = -\frac{1}{A_P} \left[T_a (x_2 - x_1) + T_b (x_1 - x_3) \right] \quad (2.2-2)$$

where

$$A_P = .5 (A_a + A_b), \quad (2.2-3)$$

A_a and A_b being zone areas.

The gradient at P is then modified so that it lies parallel to the boundary which is defined by the straight line joining points 2 and 3. This is done in the following way. A unit vector $\hat{V} = V_x \hat{i} + V_y \hat{j}$ parallels to the boundary at point P is defined as follows:

$$\hat{V} = \frac{x_3 - x_2}{\sqrt{(x_3 - x_2)^2 + (y_3 - y_2)^2}} \hat{i} + \frac{y_3 - y_2}{\sqrt{(x_3 - x_2)^2 + (y_3 - y_2)^2}} \hat{j} \quad (2.2-4)$$

where $\hat{i}$ and $\hat{j}$ are unit vectors parallel to the x and y axes. The modified components of the gradient at P then become:

Figure 6 (a)

Figure 6 (b)

Figure 6 (c)

Figure 6 (d)

FIGURE 6
TREATMENT OF BOUNDARIES

$$\left(\frac{\partial T}{\partial x}\right)_P = \left[\left(\frac{\partial T}{\partial x}\right)_P^o v_x + \left(\frac{\partial T}{\partial y}\right)_P^o v_y\right] v_x \quad (2.2-5)$$

$$\left(\frac{\partial T}{\partial y}\right)_P = \left[\left(\frac{\partial T}{\partial x}\right)_P^o v_x + \left(\frac{\partial T}{\partial y}\right)_P^o v_y\right] v_y \quad (2.2-6)$$

(b) Corner boundary point (see Figure 6 [b]).

If both zone faces common to corner point P are non-conducting, then the temperature gradient at corner point P is set equal to zero. In addition, the heat flux associated with each boundary zone face is set identically equal to zero.

Consider the case that boundary P2 is a non-conducting zone face and boundary P3 is a fixed temperature boundary. The components of the temperature gradient are initially defined at P as

$$\left(\frac{\partial T}{\partial x}\right)_P^o = \frac{1}{.5A_a} \left[T_{p3} (y_3 - y_p) + T_a (y_2 - y_3) \right] \quad (2.2-7)$$

$$\left(\frac{\partial T}{\partial y}\right)_P^o = -\frac{1}{.5A_a} \left[T_{p3} (x_3 - x_p) + T_a (x_2 - x_3) \right] \quad (2.2-8)$$

where T_{p3} is the temperature of face p3. The gradient at P is then modified so that it lies parallel to the boundary P2. This is done in the following way. A unit vector $\hat{V} = V_x \hat{i} + V_y \hat{j}$ parallel to the boundary P2 is defined as follows:

$$\hat{V} = \frac{x_p - x_2}{\sqrt{(x_p - x_2)^2 + (y_p - y_2)^2}} \hat{i} + \frac{y_p - y_2}{\sqrt{(x_p - x_2)^2 + (y_p - y_2)^2}} \hat{j} \quad (2.2-9)$$

where $\hat{i}$ and $\hat{j}$ are unit vectors parallel to the x and y axes. The modified components of the gradient at P then become

$$\left(\frac{\partial T}{\partial x}\right)_P = \left[\left(\frac{\partial T}{\partial x}\right)_P^o v_x + \left(\frac{\partial T}{\partial y}\right)_P^o v_y \right] v_x \quad (2.2-10)$$

$$\left(\frac{\partial T}{\partial y}\right)_P = \left[\left(\frac{\partial T}{\partial x}\right)_P^o v_y + \left(\frac{\partial T}{\partial y}\right)_P^o v_y \right] v_y \quad (2.2-11)$$

(2) Prescribed temperature boundaries

(a) Non-corner point (see Figure 6 [c])

The components of the gradient at P are defined as

$$\begin{aligned} \left(\frac{\partial T}{\partial x}\right)_P = \frac{1}{A_{ab}} & \left[T_a (y_2 - y_1) + T_{p2} (y_p - y_2) \right. \\ & \left. + T_{p3} (y_3 - y_p) + T_b (y_1 - y_3) \right] \end{aligned} \quad (2.2-12)$$

$$\begin{aligned} \left(\frac{\partial T}{\partial y}\right)_P = -\frac{1}{A_{ab}} & \left[T_a (x_2 - x_1) + T_{p2} (x_p - x_2) \right. \\ & \left. + T_{p3} (x_3 - x_p) + T_b (x_1 - x_3) \right] \end{aligned} \quad (2.2-13)$$

where

$$A_{ab} = .5 (A_a + A_b) \quad (2.2-14)$$

and where T_{p2} and T_{p3} are the temperatures of zone faces p2 and p3, respectively.

(b) Corner boundary point (see Figure 6[d])

The components of the gradient of P are defined as

$$\left(\frac{\partial T}{\partial x}\right)_p = \frac{1}{.5A_a} \left[T_a (y_2 - y_3) + T_{p2} (y_p - y_2) + T_{p1} (y_3 - y_p) \right] \quad (2.2-15)$$

$$\left(\frac{\partial T}{\partial y}\right)_p = -\frac{1}{.5A_a} \left[T_a (x_2 - x_1) + T_{p2} (x_p - x_2) + T_{p1} (x_3 - x_p) \right] \quad (2.2-16)$$

where A_a is the zone area and where T_{p3} and T_{p1} are the prescribed temperatures of zone faces p3 and p1, respectively.

2.3 Truncation Error and Stability

For a rectangular mesh with a constant thermal diffusivity α $\alpha = \frac{K}{\rho C_v}$, where K is the thermal conductivity, ρ is the density, and C_v is the specific heat, the difference equations have a truncation error of the following order:

$$\Delta t, (\Delta x)^2, (\Delta y)^2, \text{ for planar systems}$$

$$\Delta t, \frac{(\Delta x)^2}{y}, \frac{(\Delta y)^2}{y}, (\Delta x)^2, (\Delta y)^2 \text{ for axisymmetric systems.}$$

For the finite difference scheme to be stable, Δt , Δx , and Δy must be such that the following three inequalities are satisfied:

$$\frac{2\alpha\Delta t}{(\Delta y)^2} \leq 1 \quad (2.3-1)$$

$$\frac{2\alpha\Delta t}{(\Delta x)^2} \leq 1 \quad (2.3-2)$$

$$\frac{2\alpha\Delta t}{(\Delta x)^2 + (\Delta y)^2} \leq 1 \quad (2.3-3)$$

3.0 VALIDATION OF PROGRAM HEAT

Six transient heat conduction problems have been solved by HEAT as part of the program validation. The solutions are compared with the analytical solutions given by Carslaw and Jaeger (1959). Plots of the analytical and numerical solutions are given in Figures 7 through 15. The analytical solutions for the temperature for the six problems follow. The page references are to the second edition, Carslaw and Jaeger (1959).

3.1 One-dimensional slab - $L < z < L$

Initially at temperature T_0 .

The ends at $T = 0$ at time $t > 0$ (p. 96).

$$T = \frac{4T_0}{\pi} \sum_{n=0}^{\infty} \frac{1}{(2n+1)} e^{-(2n+1)^2 \alpha \pi^2 t / L^2} \sin \frac{(2n+1)\pi z}{L}$$

where α is the diffusivity.

3.2 One-dimensional slab $0 < z < L$

Initially at temperature zero.

$T = T_0$ at $z = 0$ and $T = 0$ at $z = +L$ at time $t \geq 0$. (pp. 102-104).

$$T = \frac{2T_0}{\pi} \sum_{n=1}^{\infty} \frac{\sin \frac{n\pi z}{L}}{n} (1 - e^{-n^2 \pi^2 \alpha t / L^2})$$

3.3 The infinite rectangular cylinder $|x| < a$, $|y| < b$ initially at temperature T_0 , and the infinite region outside it initially at zero (p. 56).

$$T = \frac{1}{4} T_0 \left(\left[\operatorname{erf} \frac{a-x}{2(\alpha t)^{1/2}} + \operatorname{erf} \frac{a+x}{2(\alpha t)^{1/2}} \right] \left[\operatorname{erf} \frac{b-y}{2(\alpha t)^{1/2}} + \operatorname{erf} \frac{b+y}{2(\alpha t)^{1/2}} \right] \right)$$

3.4 The infinite circular cylinder $r > a$ initially at temperature T_0 and the infinite region outside it initially at zero (p. 260).

ONE-DIMENSIONAL HEAT CONDUCTION

TEMPERATURE VS. DEPTH VS. TIME

FIGURE 7

THEORETICAL TEMPERATURE DISTRIBUTION

ONE-DIMENSIONAL HEAT CONDUCTION

TEMPERATURE VS. DEPTH VS. TIME

FIGURE 8

TEMPERATURE DISTRIBUTION CALCULATED BY HEAT

ONE-DIMENSIONAL HEAT CONDUCTION

TEMPERATURE VS. DEPTH VS. TIME

FIGURE 9

THEORETICAL TEMPERATURE DISTRIBUTION

ONE-DIMENSIONAL HEAT CONDUCTION

TEMPERATURE VS. DEPTH VS. TIME

FIGURE 10

TEMPERATURE DISTRIBUTION CALCULATED BY HEAT

TWO-DIMENSIONAL HEAT CONDUCTION IN AN INFINITE REGION

FIGURE 11

INFINITE RECTANGULAR CYLINDER-TEMPERATURE PROFILES AT $Y = 0.45$

TWO-DIMENSIONAL HEAT CONDUCTION IN AN INFINITE REGION

FIGURE 12

INFINITE RECTANGULAR CYLINDER-TEMPERATURE PROFILES AT $x = 0.25$

TWO-DIMENSIONAL HEAT CONDUCTION IN AN INFINITE REGION

FIGURE 13

INFINITE CIRCULAR CYLINDER-TEMPERATURE PROFILES

AXISYMMETRIC HEAT CONDUCTION IN AN INFINITE REGION

FIGURE 14

SPHERE-TEMPERATURE PROFILES

FIGURE 15
POINT SOURCE

$$T = \frac{T_0}{2\alpha t} e^{-r^2/4\alpha t} \int_0^a e^{-x^2/4\alpha t} I_0 \left[\frac{rx}{4\alpha t} \right] x dx$$

where I_0 is the modified Bessel function.

3.5 The spherical region $r < a$ initially at temperature T_0 and the infinite region outside it initially at zero (p. 257).

$$T = \frac{1}{2} T_0 \left[\operatorname{erf} \frac{r+a}{2(\alpha t)^{1/2}} - \operatorname{erf} \frac{r-a}{2(\alpha t)^{1/2}} - \frac{2(\alpha t)^{1/2}}{r\pi} \left(e^{-(r-a)^2/4\alpha t} - e^{-(r+a)^2/4\alpha t} \right) \right]$$

3.6 The infinite region initially at temperature zero. A point source of strength Q is placed at the origin at time $t = 0$ (p. 261).

$$T = \frac{Q}{4\pi\alpha r} \operatorname{erfc} \frac{r}{\sqrt{4\alpha t}}$$

ACKNOWLEDGEMENTS

The numerical formulation used in HEAT is almost identical to that used in PISCES 2DL (see Jardin, et al., 1972).

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APPENDIX 2

BOREHOLE DECREPITATION:
A STUDY OF COUPLED NON-LINEAR THERMO-MECHANICAL RESPONSE AROUND A CANISTER

APPENDIX 2

BOREHOLE DECREPITATION:
A STUDY OF COUPLED NON-LINEAR THERMO-MECHANICAL RESPONSE AROUND A CANISTER1.0 INTRODUCTION

On the canister scale, the combination of thermal and in situ stresses could cause decrepitation; i.e., fragmentation and disintegration, of the basalt and some change in the thermal properties of the basalt. If this change in rock structure accompanying decrepitation produces a lowering of the effective thermal diffusivity of the basalt then heat transfer from the canister to the basalt will be hindered. This could result in "thermal runaway" whereby the temperature of the canister increases to exceed some allowable canister temperature. Other mechanisms could contribute to a condition leading to thermal runaway; for example, changes in moisture content of the basalt and changes in connection paths for air flow around the canister. However, these were not considered in this study.

In this study an attempt has been made to analyze the coupled heat flow, mechanical response around the canister. The coupling is via a volumetric strain-dependent thermal conductivity. Other forms of coupling could be used and more refined analysis presented; this analysis allowed some rational review of the types of "material properties" required and what types of coupling could be analyzed using existing code capabilities. The STEALTH¹

explicit finite difference code was used for this analysis as it is ideal for these highly non-linear coupled problems. Later, if necessary, two- or three-dimensional analysis could be performed using the same code.

2.0 DESCRIPTION OF MODEL

2.1 Geometry and Boundary Conditions

STEALTH was applied to the evaluation of the thermo-mechanical interaction of a waste canister within a borehole by assuming certain symmetry conditions. For this problem an axisymmetric one-dimensional analysis about a single canister was performed in which the flux was assumed to flow only in the radial direction away from the center line of the canister. This analysis is appropriate for very short times when the temperature and induced stresses are relatively independent of neighboring heat sources.

A finite-difference mesh for this one-dimensional axisymmetric problem is shown in Fig. 1. The mesh contains 21 zones with the canister heat source located in the two zones between grid points 1 and 3. The remaining zones were given the properties of basalt.

The outside radius of the cylinder was 5 m since canisters are considered to be at approximately 10 m spacing. A 0.4-m diameter canister with a thermal output of 1 kw (thermal density of 1.59 kw/m^3) is concentric with the cylinder.

FIGURE 1

FINITE DIFFERENCE MESH FOR ONE-DIMENSIONAL
AXISYMMETRY WITH BOUNDARY CONDITIONS

The elastic and thermal properties for the basalt rock and the canister used in the cylinder model are shown in the table below. The elastic properties of the canister were reduced by 1/5 of their typical values and the thermal properties by 1/2 to simulate a mixed zone of air and heat source.

Elastic and Thermal Properties

	<u>Basalt</u>	<u>Canister</u>
Bulk Modulus (Pa)	0.268×10^{11}	0.536×10^{10}
(psi)	0.389×10^7	0.777×10^6
Shear Modulus (Pa)	0.197×10^{11}	0.402×10^{10}
(psi)	0.286×10^7	0.583×10^6
Mass Density (kg/m^3)	2900.	4700.
Heat Capacity ($\text{J}/(\text{m}^3 \cdot ^\circ\text{C})$)	2.987×10^6	1.210×10^6
Thermal Conductivity (Watts/($\text{m} \cdot ^\circ\text{C}$))	1.84	0.96
Thermal Expansion Coefficient ($^\circ\text{C}^{-1}$)	5.4×10^{-6}	5.4×10^{-6}

A radial compressive stress of 28.42 MPa (4122 psi) was applied to the outer boundary of the cylinder. This boundary condition simulates an in situ pre-heating horizontal stress which is taken to be equal to a vertical stress at a depth of 1000 m. This stress condition plus the assumption of zero axial displacement would be appropriate for a deeply buried canister.

Since the study was for short time periods, the outer boundary of the cylinder was considered as heat flux free. Ambient temperature for the analysis was chosen to be 0°C.

2.2 Constitute Relationships

The thermal and mechanical non-linear response was selected to simulate the initiation of a zone of decrepitation in the basalt immediately surrounding the canister as the temperature of the rock rises. Thermal conductivity of the rock was considered to be a function of the volumetric strain. That is, dilatation in the rock was assumed to produce a corresponding decrease in the rock's thermal conductivity. The dependence of thermal conductivity, k , on volumetric strain Δ was assumed to be of the form:

$$K = K_0 (1 - .75 (1 - e^{-\lambda \Delta})) \quad (2.2-1)$$

where k_0 is the initial conductivity, and λ is a dimensionless constant chosen such that the thermal conductivity of the first rock zone adjacent to the canister dropped to at least 1/2 of its original value within the time frame of the study. Note that the thermal conductivity was arbitrarily chosen to approach 1/4 of its original value as Δ approaches infinity. Laboratory results are needed to provide a better approximation for this relationship.

The mechanical behavior of the basalt was based upon elastic-perfectly plastic failure theory using the von Mises yield criteria. For this criterion, yield occurs when the octahedral shear stress reaches a value characteristic of the material. A consequence of the von Mises

yield condition is that hydrostatic pressure has no effect on plastic deformation and that dilatancy of the material does not occur. A more realistic yield criterion for rock would include the effects of changing hydrostatic pressure and resulting volumetric strain. Work toward including these effects in the STEALTH code using the Drucker-Prager yield criterion with a non-associative flow rule is currently in progress.

Two case studies were made for comparison. In Case A, elastic mechanical properties and constant thermal properties of the rock as given in the table were used to describe the complete material behavior. In Case B, the non-linear material behavior described above was used. Values for the non-linear relationships of Case B were based upon the equilibrium stress state of the cylinder when subjected only to the compressive radial stress on the outer boundary. The initial thermal conductivity was taken to be a constant value of 1.84 watts/(m³-°C) throughout the model. A value of 5000 was determined for the dimensionless constant λ . The yield stress of the basalt was set at 23 MPA (3335 psi), so that failure would occur within the time frame of the study.

3.0 COMPARISON OF RESULTS

A time range of 28 days (1500 computer cycles with a time step of 1600 sec. per cycle) was sufficient for the model to become reasonably developed and still be independent of the influence of neighboring heat sources. The results are presented in the form

of "snap shot" plots taken of the model at specific times. The plots are given in Figs. 2 through 14.

For both Cases A and B, the horizontal stress was applied first and stresses in the model were allowed to develop to their static equilibrium values before the canister heat was turned on. Static equilibrium was established by 500 cycles, at which time the canister heaters were turned on.

The stress state in the model prior to heating is shown by the radial stress, hoop stress and vertical stress plots in Figs. 2, 3 and 4, respectively. The reduced elastic properties in the canister zones cause the center of the cylinder to be less competent than the surrounding material and thus stresses are less at the center. If the properties were further reduced, the model would approach a cylinder with a concentric circular hole. As an indication of the validity of the model, the analytical plane strain solution is given for the equilibrium stress state of a cylinder with a 0.4 m. diameter concentric hole and subjected to 28.42 MPa (4122 psi) compressive radial stress in Figs. 2, 3 and 4.

It should be remarked at this point that for a plane strain analysis of an infinitely long circular cylinder with a concentric hole, the volumetric strain developed purely under an elastic stress state is constant throughout. This can be seen by studying the equations for stress and strain in a long cylinder as developed by Timoshenko and Goodier.² For the model analysis, the volumetric strain due to the compressive radial stress was determined to be

FIGURE 2

STRESS PROFILE PRIOR TO HEATING - CASES A AND B
(Radial stress versus radial distance at cycle 500 - stress is positive in tension.)

FIGURE 3

STRESS PROFILE PRIOR TO HEATING - CASES A AND B
(Hoop stress versus radial distance at cycle 500 -
stress is positive in tension.)

FIGURE 4

STRESS PROFILE PRIOR TO HEATING - CASES A AND B
(Axial stress versus radial distance at cycle
500 - stress is positive in tension.)

FIGURE 5

THERMALLY INDUCED VOLUMETRIC STRAIN VERSUS RADIAL DISTANCE AT CYCLE 2000
(Strain is positive in dilatation relative to initial volumetric strain
of -8.5×10^{-4} .)

FIGURE 6

CONDUCTIVITY VERSUS RADIAL DISTANCE AT CYCLE 2000 - CASE B

FIGURE 7

TEMPERATURE VERSUS RADIAL DISTANCE AT CYCLE 2000 - CASE A

FIGURE 8

TEMPERATURE VERSUS RADIAL DISTANCE AT CYCLE 2000 - CASE B

FIGURE 9

RADIAL STRESS VERSUS RADIAL DISTANCE AT CYCLE 2000 - CASE A
(Stress is positive in tension.)

FIGURE 10

HOOP STRESS VERSUS RADIAL DISTANCE AT CYCLE 2000 - CASE A
(Stress is positive in tension.)

FIGURE 11

AXIAL STRESS VERSUS RADIAL DISTANCE AT CYCLE 2000 - CASE A
(Stress is positive in tension.)

FIGURE 12

RADIAL STRESS VERSUS RADIAL DISTANCE AT CYCLE 2000 - CASE B
(Stress is positive in tension.)

FIGURE 13

HOOP STRESS VERSUS RADIAL DISTANCE AT CYCLE 2000 - CASE B
(Stress is positive in tension.)

FIGURE 14

AXIAL STRESS VERSUS RADIAL DISTANCE AT CYCLE 2000 - CASE B
(Stress is positive in tension.)

-8.5×10^{-4} (strain is considered positive in dilatation). As a comparison, the volumetric strain from the analytical analysis for the cylinder with the concentric hole was found to be -7.8×10^{-4} .

Thus, strain-dependent thermal conductivity in the rock is constant throughout the rock even after the introduction of the hole. This, of course, does not allow for any discontinuities in the rock structure.

Dilatation and contraction in the rock due to the thermal stresses and failure* were measured relative to the initial mechanically induced volumetric strain. Fig. 5 shows a plot of thermally induced volumetric strain for Case B 1500 cycles after heating. During the heating period the first rock zone adjacent to the canister was allowed to yield. The relative dilatation was highest in this zone reaching a value of 5.24×10^{-4} at the end of the study time. The corresponding strain-dependent thermal conductivity after 1500 cycles of heating is plotted in Fig. 6. As indicated by this plot, the conductivity drops to a low of $0.56 \text{ watts}/(\text{m}^3 - ^\circ\text{C})$ in the first rock zone adjacent to the canister at this time.

The effects on temperature distribution in the model due to the non-linear material behavior can be seen by comparing the temperature profile for Case A Fig. 7, with that for Case B, Fig. 8. After 1500 cycles of heat, the peak temperature in the canister is 35°C hotter (an increase of 60%) for the non-linear case than for

*For this analysis, failure resulted in no volume change, since the von Mises yield condition was used.

the linearly elastic case. This temperature buildup and inability of the model to conduct heat away from the source can be attributed to the growth of the zone of decrepitation in the rock.

The stress state after 1500 cycles of heat is given for Case A by Figs. 9, 10 and 11 and for Case B by Figs. 12, 13 and 14. The thermally induced radial, hoop and axial stresses all increase in compression for both cases. Note that all the stresses are higher in compression for Case B than for Case A. This increase is attributed to the decrease in thermal conductivity and subsequent higher rock temperatures for Case B. The stresses are also modified somewhat by the yielding of the first basalt zone adjacent to the canister.

4.0 DISCUSSION

The results of the model analysis indicate that the presence of a zone of decrepitation in the rock around a waste canister can reduce the conductivity of the heat away from the canister and cause a heat buildup in the canister over a short period of time. The growth of the decrepitation zone was analogous to the yield zone for the rock with the reduction in thermal conductivity a function of the volumetric strain in the failed rock.

For this analysis the volumetric expansion was entirely temperature dependent; dilatation associated with yield was not included. In reality, yield-dependent dilatation may be much larger than that induced thermally. Further, the thermal conductivity-volumetric strain

relationship may not be based upon the total volume change but only upon that induced by yield. Thus, the form of the thermal conductivity mechanical response could be quite complex and requires more detailed laboratory and analytical study.

Since the material behavior model was not based on laboratory or known basalt properties, such information is not available, a worst case study for temperature buildup in the canister could not be made. However, it should be noted that STEALTH has the capability to handle more complicated constitutive models. Therefore, as the non-linear behavior of thermal and mechanical properties of the basalt become more fully defined, a more detailed analysis can be made with the STEALTH code.

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APPENDIX 3

DIFFUS2, A ONE-DIMENSIONAL ANALYSIS OF A WASTE REPOSITORY

APPENDIX 3

DIFFUS2, A ONE-DIMENSIONAL ANALYSIS OF A WASTE REPOSITORY

1.0 INTRODUCTION

The areal extent of a radioactive waste repository is expected to be large with respect to its depth below the surface. It would seem reasonable, therefore, to approximate the repository as an infinite plane, lying parallel to the ground surface, and at which heat is generated at a rate depending upon the age of the radioactive waste stored. Under these circumstances, a repository may be analyzed by solving the one-dimensional diffusion equation with a heat source term included.

This appendix discusses the solution of the one-dimensional diffusion equation, presents the results of a series of computer runs made using a simple computer program and, finally, comments on the validity of treating a repository as a one-dimensional problem.

2.0 THE ONE-DIMENSIONAL DIFFUSION EQUATION AND ITS SOLUTION

The governing equation for one-dimensional heat diffusion is:

$$c\rho \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(K \frac{\partial T}{\partial x} \right) + A \quad (2.0-1)$$

where $T = T(x,t)$ is the temperature

$K = K(x,t)$ is the thermal conductivity

$\rho = \rho(x,t)$ is the density

$c = c(x,t)$ is the specific heat

$A = A(x,t)$ is the heat generation (per unit time per unit volume)

If we discretize this equation in time and space to obtain a finite difference form the solution is simple even for non-homogeneous materials and

varying heat generation rates.

Let the figure represent the discretization in space. Temperature will be calculated for each point $j-1$, j , $j+1$ etc., at time i , $i+1$ etc. The spacing between calculation points is assumed to be a constant Δx and the region length Δx centered around each point will be referred to as a zone.

Integrating the diffusion equation over one zone for one time step of length Δt gives:

$$\int_{x_-}^{x_+} \int_t^{t + \Delta t} c \rho \frac{\partial T}{\partial t} dt dx = \int_t^{t + \Delta t} \int_{x_-}^{x_+} \frac{\partial}{\partial x} K \frac{\partial T}{\partial x} dx dt + \int_t^{t + \Delta t} \int_{x_-}^{x_+} A dx dt \quad (2.0-2)$$

Assuming that the temperature varies linearly from point to point and that the heat generation rate is constant over any time step then:

$$c_j \rho_j (T_j - T_j^o) \Delta x = [K_{x_+} \frac{(T_{j+1} - T_j)}{\Delta x} - K_{x_-} \frac{(T_j - T_{j-1})}{\Delta x}] \Delta t + A \Delta t \Delta x \quad (2.0-3)$$

where T_j^o is the temperature at point j at the previous time and K_{x_+} and K_{x_-} are the thermal conductivities between points $j+1$ and j and j and $j-1$ respectively. This equation may be rewritten as:

$$T_j = T_j^o + \frac{\Delta t}{\Delta x^2 c_j \rho_j} [K_{x_+} (T_{j+1} - T_j) - K_{x_-} (T_j - T_{j-1})] + \frac{A \Delta t}{c_j \rho_j} \quad (2.0-4)$$

In this equation the derivatives of temperature with respect to distance might be evaluated at the start of the time step, at the end of the time step

or at some intermediate time. Assume that the value of the temperature is obtained from some weighting factor ω from the following expression:

$$\omega T + (1 - \omega) T^o \quad (2.0-5)$$

Substituting this into the finite difference representation of the diffusion equation:

$$T_j = T_j^o + \frac{\Delta t}{\Delta x^2 c_j \rho_j} [\omega (K_{x+} (T_{j+1} - T_j) - K_{x-} (T_j - T_{j-1})) + (1 - \omega) (K_{x+} (T_{j+1}^o - T_j^o) - K_{x-} (T_j^o - T_{j-1}^o))] + \frac{A \Delta t}{\rho_j c_j} \quad (2.0-6)$$

The method of solution will now depend upon the value of ω selected. For $\omega = 0$, the equation is explicit and may be solved using a simple time stepping algorithm. For $\omega = 1$ the equation is fully implicit and a solution must be obtained by solution of a set of equations. For $\omega = 0.5$ the Crank-Nicolson formulation is obtained.

For the purposes of this work, it is convenient to use the explicit formulation. Introducing the superscript i to represent time the equation becomes:

$$T_j^{i+1} = T_j^i + \frac{\Delta t}{\Delta x^2 c_j \rho_j} [K_{x+} (T_{j+1}^i - T_j^i) - K_{x-} (T_j^i - T_{j-1}^i)] + \frac{A^{i+1} \Delta t}{c_j \rho_j} \quad (2.0-7)$$

where the heat generated has been evaluated at the end of the time step.

In this equation it has been assumed that the density and specific heat are constant over any zone. If the thermal conductivity is similarly assumed to be constant over a zone then the conductivities K_{x+} and K_{x-} must be calculated from the zone conductivities. In the computer program, these values are calculated as the harmonic means of the zone conductivities.

$$K_{x+} = \frac{2.0 K_{j+1} K_j}{K_{j+1} + K_j} \quad (2.0-8)$$

and similarly for K_{x-} .

This gives a much better approximation than taking the average value. For example, at a perfectly insulated boundary the harmonic mean gives an inter-zone conductivity of zero. The boundary condition is thus automatically satisfied. Such would not be the case if the arithmetic mean of the conductivities were used.

Once the temperature profile at any time step has been determined, then the energy content of the rock mass and the surface displacement may be calculated.

$$\text{Energy content} = \int_0^{\infty} c \rho T dx \quad (2.0-9)$$

$$\text{Surface displacement} = \int_0^{\infty} \alpha T dx \quad (2.0-10)$$

where T , the temperature change, is some function of distance from the surface and α is the coefficient of linear thermal expansion. The equation for surface displacement assumes that there will be no resistance to lateral strain resulting from temperature changes.

3.0 VALIDATION OF THE ONE-DIMENSIONAL DIFFUSION MODEL

A report prepared by St. John⁽¹⁾ and submitted to the Office of Waste Isolation, Union Carbide Corporation, contains results of analyses of spent unprocessed fuel (SURF) and high-level waste (HLW) repositories in a homogeneous salt mass. Model data were as follows:

Depth of repository	2000 ft.
Areal dimensions	6204 ft. square
Thermal loading density	150 kw/acre
Material Properties:	
Thermal conductivity	4.325 watts/m°C
Specific heat	920 J/kg°C
Density	2100 kg/m ³
Linear expansion coefficient	40 x 10 ⁻⁶ /°C

The thermal loading densities for both cases were 150 kw/acre (37 J/s m²). Constituents of the decaying heat generation components, expressed as the energy input per m² were:

SURF	$0.2801 \times e^{-2.3 \times 10^{-5}t}$	HLW	$0.0074 \times e^{-1.5 \times 10^{-5}t}$
	$0.561 \times e^{-9.95 \times 10^{-5}t}$		$0.0025 \times e^{-7.49 \times 10^{-5}t}$
	$5.206 \times e^{-1.75 \times 10^{-3}t}$		$0.111 \times e^{-1.12 \times 10^{-3}t}$
	$25.10 \times e^{-2.163 \times 10^{-2}t}$		$0.2631 \times e^{-2.34 \times 10^{-3}t}$
	$1.869 \times e^{-4.014 \times 10^{-2}t}$		$31.40 \times e^{-2.42 \times 10^{-2}t}$
	$4.051 \times e^{-2.915 \times 10^{-1}t}$		$2.865 \times e^{-1.17 \times 10^{-1}t}$
			$2.391 \times e^{-4.83 \times 10^{-1}t}$

Runs were completed using a constant mesh size of 12.5 m and time step sizes of both 0.5 and 2.0 years. Comparisons were then made between temperatures calculated by the two models at a point midway between the repository

horizon and the surface. The figure shows that agreement is good over relatively short time periods, but is poor after around 1000 years. Some results providing validation of DIFFUS2 are also given in the table below. Short time differences between these results may be attributed to the fact that the three-dimension model reported⁽¹⁾ used a limited number of concentrated heat sources distributed across the plane of the repository. Long-term differences arise because of lateral heat conduction in the three-dimensional model.

Time (years)	Analytical 3D Solution		DIFFUS2	
	Spent Fuel °F	High Level Waste °F	Spent Fuel °F	High Level Waste °F
100	78.3	77.9	77.3	77.1
500	138.1	107.5	136.8	107.4
1000	161.9	104.5	166.8	107.4

REFERENCE

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TEMPERATURES 1000 FEET ABOVE REPOSITORIES IN HOMOGENEOUS SALT
COMPARISON OF ONE- AND THREE-DIMENSIONAL SOLUTIONS
(150 KW/ACRE)

APPENDIX 4

THE EFFECT OF AQUIFER FLOW ON THE HEAT TRANSFER
NEAR A NUCLEAR WASTE REPOSITORY

APPENDIX 4

THE EFFECT OF AQUIFER FLOW ON THE HEAT TRANSFER
NEAR A NUCLEAR WASTE REPOSITORY1.0 INTRODUCTION

The consequences of groundwater flow heat transfer interaction are important considerations in the design of a radioactive waste repository in basalt. These two phenomena are coupled in most situations; that is, neither can be simulated accurately unless the effect of the other is included in the model. This appendix examines the influence of groundwater flow, that is confined to relatively thin aquifers, on the heat transport around a full-scale repository. This is a long term, regional problem because temperature changes do not occur at the aquifer level for hundreds of years after waste emplacement.

One factor which may limit the size or allowable gross thermal loading of a waste repository is the repository impact on the regional groundwater temperatures. To demonstrate a capability to examine this sort of problem a simple repository, two aquifer system was modeled. The aquifers in the model correspond to the Mabton Interbed and the Vantage Sandstone located in the Pasco Basin.

2.0 MODEL DESCRIPTION

The finite element code (BASFEH) used to model this heat transfer-fluid flow problem is a modified version of the code written by Nelson.⁽¹⁾ In its original form, this code had the capability to model plane or axisymmetric heat transfer problems

with inhomogeneous, non-isotropic materials. To be applicable to the problem at hand, the code required alterations which would allow exponentially decaying heat sources and heat transfer due to forced convection.

To approximate the magnitude of heat transfer due to forced convection, a special two-node "aquifer" finite element was developed. Figure 1 shows how a series of such aquifer elements is included in the solid element mesh. These aquifer elements have the following characteristics:

- (1) A real thickness of zero, so
- (2) The element has zero heat capacity,
- (3) An "aquifer" thickness of W ,
- (4) An "aquifer fluid flowing with a velocity of V , having a heat capacity of C .

The power input to any node i , connected to adjacent nodes $i-1$ and $i+1$ by two aquifer elements, is defined as:

$$P_i = -CVW \left[\frac{T_i - T_{i-1}}{2} + \frac{T_{i+1} - T_i}{2} \right], \quad (2.0-1)$$

$$P_i = CVW \left[\frac{T_{i-1} - T_{i+1}}{2} \right].$$

Thus, there is a positive power input at any node for which the nearest upstream node has a higher temperature than the nearest downstream node.

With these modifications BASFEH couples the processes of heat transfer and forced convection, but does not consider any change in the flow regime due to natural convection cells. Also, considering the zero thickness, zero heat capacity properties of the aquifer element, the code should only be used to model relatively thin, distinct regions of fluid flow.

A - Denotes an Aquifer Element

FIGURE 1

AQUIFER ELEMENTS INCLUDED IN THE SOLID ELEMENT MESH

3.0 CODE VERIFICATION

To verify the accuracy of both the heat conduction and forced convection phases of the BASFEH code comparisons were made with a one dimensional heat conduction code DIFFUS, and with a closed form one dimensional solution for the heat conduction, heat convection problem.

DIFFUS is a one dimensional implicit formulation of the heat conduction equation developed by St. John.⁽²⁾ This model simulates the vertical section of a repository and assumes that there is no lateral heat flow. The repository modeled by BASFEH was two-dimensional hence the comparison of the one dimensional and two-dimensional codes is valid only near the center of the repository and for a limited distance above and below it. Figure 2 shows a comparison of the temperature changes versus distance above

FIGURE 2
COMPARISON OF BASFEH AND DIFFUS RESULTS

the repository from the two codes. The input data and mesh layout for this run are discussed in the following section. The results shown in Figure 2 are for 1000 years after waste emplacement. This figure shows minor differences between the results near the repository but identical results for more distant points.

Validation of the forced convection aspect of the BASFEH code was accomplished through comparison with a problem having a closed form solution. Ratigan⁽³⁾ used the solution of the one-dimensional convective diffusion problem⁽⁴⁾ to validate a similar finite element code. The problem as modeled here had the following boundary conditions:

$$T(0,t) = 1, \quad (3.0-1)$$

$$T(\infty,t) = T(x,0) = 0. \quad (3.0-2)$$

The finite element mesh used for the simulation is shown in Figure 3, along with a comparison of the analytical solution and the BASFEH results. The figure reflects a good correspondence between the results.

4.0 MESH LAYOUT AND INPUT DATA

The mesh used to model half of a repository is shown in Figure 4 which also shows the geologic cross section, the position of heat sources and the two horizontal aquifer layers. Half the repository was modeled because the problem is geometrically symmetrical, but due to the fluid flow from left to right, the problem is not completely symmetric. Across the line of geometric symmetry there will be no heat flow provided that the aquifer does not transfer any heat laterally at this line. Under the conditions analyzed in this appendix this is true for most cases. This condition is discussed further after the results are presented.

In Figure 4 the plotted element members denote the location of the aquifer elements. Listed in Table 1 are the material properties used to represent the sandstone and basalt. The temperatures computed for the source nodes should not be considered representative of the true room-scale temperatures because of the coarse mesh and the absence of 'rooms' in the mesh. Boundary conditions were constant temperatures along the top surface and no-flow along all other boundaries.

Nodal power inputs were calculated on the basis of a gross thermal loading of 100 KW/acre with component proportions and half-lives selected to match the thermal output of 10-year-old

FIGURE 3

COMPARISON OF BASFEH AND THE ANALYTICAL SOLUTION OF THE CONDUCTION/CONVECTION PROBLEM

FIGURE 4

FINITE ELEMENT MESH

TABLE 1
MATERIAL PROPERTIES

	Density (kg/m ³)	Specific Heat (J/kg - °C)	Thermal Conductivity (watts/m - °k)
Sandstone	1930	1030	0.46
Basalt	2900	1030	1.85

spent fuel. A six-component source formulation was used to provide adequate representation of the heat generation out to 5000 years. The proportion, half-life, and decay constant of each component are listed in Table 2. The tabulated power output of spent fuel

TABLE 2
EXPONENTIALLY DECAYING SOURCE COMPONENTS

	Proportion	Half-Life (years)	Decay Constants (years ⁻¹)
1	0.00756	30140	2.3×10^{-5}
2	0.0151	6970	9.95×10^{-5}
3	0.1404	396	1.75×10^{-3}
4	0.677	32.0	2.163×10^{-2}
5	0.0504	17.2	4.014×10^{-2}
6	0.1093	2.38	2.915×10^{-1}

waste is compared to the computed output of the six-component source in Figure 5, and it is clear that the two match closely.

Published temperature logs of boreholes located on the Hanford Site⁽⁵⁾ indicate a regional temperature gradient of $0.04^{\circ}\text{C}/\text{meter}$. However, temperatures at the repository depth vary about 40°C from borehole to borehole. Borehole DC-1, located near the center of the site, was chosen to provide the repository depth temperatures for use here. The initial temperature distribution for the finite element mesh was computed from the 1100m depth temperature of 55°C , and the $0.04^{\circ}\text{C}/\text{m}$ gradient. It should be noted that the other sections of this report use a repository depth temperature of 67°C .

Aquifer properties were estimated from data presented in Reference 5. A base case flow velocity of $1.0 \times 10^{-7} \text{m/sec}$ was calculated from a permeability of 9.0m/day and a head gradient of 1m/km . Simulations were then run using flow velocities of 0, $1 \times 10^{-7} \text{m/sec}$, and $1 \times 10^{-6} \text{m/sec}$, with the same velocity used for both aquifers. Similarly, an aquifer width of 3.6m was used for both aquifers. Aquifer fluid properties used were those of water (i.e., Sp. heat = $4190 \text{ J/kg} \cdot ^{\circ}\text{C}$, density = 990 kg/m^3).

5.0 RESULTS OF THE FINITE ELEMENT RUNS

The results of the no flow simulation are summarized in Figure 6, where temperatures at the repository level and at aquifers 1 and 2 are plotted versus time. Repository level temperatures reach a peak value at about 100 years, and

FIGURE 5

COMPARISON OF THE SIX-COMPONENT EXPONENTIALLY DECAYING
SOURCE AND THE TABULATED INPUT OF 10-YEAR-OLD SPENT
FUEL

FIGURE 6

TEMPERATURE VERSUS TIME PLOT FOR THE REPOSITORY LEVEL, AQUIFER 1 AND AQUIFER 2

maintain this peak until about 400 years. Aquifer 2, located 245m above the repository, is not appreciably affected by the repository until 300 years. Considering the shape of the temperature-time curve for Aquifer 2 it appears that the peak temperatures in the aquifer will be about 90°C, and that the peak will endure for several thousand years. Aquifer 1, located 490m above the repository, shows no significant temperature increase until 1000 years after waste emplacement. The shape of the temperature-time curve for Aquifer 1 indicates that the peak temperature will be slightly less than the Aquifer 2 peak of 90°C.

Temperature contours for selected times during the no flow simulation are presented in Figure 7. A number of these contour plots have rough or discontinuous contours (e.g. 1000-year contour plot). These perturbations are the result of a computer routine whose purpose it is to interpolate a regularly spaced data grid from the irregular finite element mesh data. The resulting regularly gridded data values are very dependent upon the location of the irregular grid points. In viewing these plots, it is also important to remember that the left hand edge is a line of 'symmetry.'

These plots reveal that the major influence of the repository is confined to the rock directly above and below the repository, while the rock to the side of it is generally unaffected.

The 1×10^{-7} m/sec base case flow simulation yields virtually the same results as the no-flow case. Temperature contours at times 1000 years and 5000 years for the base flow simulation are shown in Figure 8. The only noteworthy difference between the results of the

FIGURE 7
TEMPERATURE CONTOURS FOR SELECTED TIMES DURING THE NO-FLOW SIMULATION (°C)

TEMPERATURE CONTOURS FOR TIME= 100. YEARS

TEMPERATURE CONTOURS FOR TIME= 500. YEARS

HORIZONTAL AND VERTICAL SCALES ARE EQUAL

Figure 7 (continued)

TEMPERATURE CONTOURS FOR TIME= 1000. YEARS

HORIZONTAL AND VERTICAL SCALES ARE EQUAL

TEMPERATURE CONTOURS FOR TIME= 2000. YEARS

Figure 7 (continued)

TEMPERATURE CONTOURS FOR TIME= 3000. YEARS

TEMPERATURE CONTOURS FOR TIME= 4000. YEARS

HORIZONTAL AND VERTICAL SCALES ARE EQUAL

Figure 7 (continued)

HORIZONTAL AND VERTICAL SCALES ARE EQUAL

TEMPERATURE CONTOURS FOR TIME= 5000. YEARS

Figure 7 (continued)

TEMPERATURE CONTOURS FOR TIME= 1000. YEARS

TEMPERATURE CONTOURS FOR TIME= 5000. YEARS

HORIZONTAL AND VERTICAL SCALES ARE EQUAL

FIGURE 8

TEMPERATURE CONTOURS FOR SELECTED TIMES DURING THE BASE FLOW SIMULATION ($^{\circ}\text{C}$)

no-flow and base flow case is a 2-5°C temperature increase at nodes above and to the right of the end of the repository.

On the other hand, the base flow times 10 case of 1×10^{-6} m/sec shows a considerable effect on temperatures due to aquifer flow. Figure 9 consists of temperature contours for 1000-5000 years for this flow case. From these plots, it is easy to determine the extent of the heat transfer due to convection. No noticeable effect of convective heat transfer is evident until 2000 years, but by 5000 years considerable portions of the rock to the right of the repository have been heated. In some cases, the temperature increase is more than 20°C.

Tables 3 and 4 illustrate the downstream extent of the effect of the repository. The values listed in Table 3 are the ratio of the length of the lower aquifer having a temperature increase of more than 30°C divided by the repository half-width of 1100 meters. There is little downstream effect resulting from a base case flow rate, while the base flow x 10 results indicate an affected length of 1.5 times the repository half-width, after 5000 years.

Table 4 shows the extent of 15°C, 30°C, and 40°C temperature increases for the lower aquifer after 5000 years. Again, there is little effect due to a base case flow rate. For the base flow x 10 case, the 15°C temperature increase extends to the edge of the mesh, 1100m past the edge of the repository. Although this is a significant departure from the no flow temperature distribution, it is probably not enough to markedly affect the stresses in that region. Further, a temperature increase of that magnitude and extent will not have any impact on the regional water supply. These

TEMPERATURE CONTOURS FOR TIME= 1000. YEARS

TEMPERATURE CONTOURS FOR TIME= 2000. YEARS

HORIZONTAL AND VERTICAL SCALES ARE EQUAL

FIGURE 9

TEMPERATURE CONTOURS FOR SELECTED TIMES DURING THE BASE FLOW X 10 SIMULATION ($^{\circ}\text{C}$)

TEMPERATURE CONTOURS FOR TIME= 3000. YEARS

TEMPERATURE CONTOURS FOR TIME= 4000. YEARS

HORIZONTAL AND VERTICAL SCALES ARE EQUAL

Figure 9 (continued)

HORIZONTAL AND VERTICAL SCALES ARE EQUAL

TEMPERATURE CONTOURS FOR TIME = 5000. YEARS

Figure 9 (continued)

TABLE 3

PORTION OF THE LOWER AQUIFER WITH A TEMPERATURE
INCREASE GREATER THAN 30°C

(i.e., length of affected aquifer/1100 m)

Time (Years)	1000	2000	3000	4000	5000
No Flow	0	0.77	0.84	0.84	0.88
Base Flow	0	0.84	0.88	0.94	0.94
Base Flowx10	0	1.11	1.27	1.44	1.55

TABLE 4

PORTION OF THE LOWER AQUIFER WITH A TEMPERATURE
INCREASE GREATER THAN 15°C, 30°C, 40°C FOR TIME = 5000 YEARS

(i.e., length of affected aquifer/1100 m)

ΔT	15°C	30°C	40°C
No Flow	1.12	0.88	0.50
Base Flow	1.27	0.94	0.60
Base Flowx10	2	1.55	1.0

conclusions are, of course, very dependent on the aquifer flow rates and thicknesses used in the simulation.

The no heat flow boundary condition at the line of geometric symmetry can be examined knowing the temperature distribution for the problems analyzed. As noted earlier, the addition of fluid flow in the aquifers destroys the strict symmetry of the problem. However, for some times and flow rates the symmetric formulation of the problem will yield the same result as the non-symmetric formulation. The controlling factor is illustrated in Figure 10, where temperature contours are shown for a non-symmetric formulation. In Figure 10, contours 1, 2, and 3 are for the same temperature level at increasing times. The action of the aquifer fluid is to depress temperatures on the upstream side of the repository. This causes a separation between the no-flow contours and the flow contours. The leading edge of this separation could be called the separation point (SP) and it is when this separation point moves across the repository center line that the symmetric approximation is no longer valid. Referring to Figure 10, the symmetric approximation is well grounded for times 1 and 2, but not for time 3. From examining the 1×10^{-6} m/sec flow case contours (Figure 9) it is possible to conclude that the 4000 and 5000 year results may be invalid due to the above argument.

FIGURE 10

TIME HISTORY OF A TEMPERATURE CONTOUR AFFECTED BY AQUIFER FLOW

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APPENDIX 5

TWO-DIMENSIONAL COUPLED THERMAL AND
FLUID FLOW ANALYSIS IN POROUS MEDIA

APPENDIX 5

TWO-DIMENSIONAL COUPLED THERMAL AND
FLUID FLOW ANALYSIS IN POROUS MEDIA1.0 GENERAL DESCRIPTION

The mathematical model is based upon the classical equations of porous media flow with temperature-dependent water properties. It is suitable for both steady- and unsteady-state flow. The model also allows for anisotropy of hydraulic conductivities and variation of the hydrologic parameters over space and time. In its present form, it is a two-dimensional model and a solution to the governing mathematical equations is obtained by a combination of the alternating-direction-implicit technique with integrated finite differences. The resulting algorithm is numerically stable and possesses an accuracy of the second-order in the space and of the first-order in the time domain. The program accepts an irregular two-dimensional grid over which the various material and fluid properties are defined. Most input data are read in free format and may be modified at any stage of the run. The time step and maximum time are set by the user. Solutions to the equations yield pressure, velocity, and temperature values every time step at each grid cell. Output options are extremely flexible and almost completely user-determined. Thermal conductivity, heat capacity, permeability, density, and viscosity values over the entire grid may be displayed, and calculated pressure, temperature, and velocity values may be printed as frequently as desired during processing. Stream function values based on final fluid velocities are computed and may also be displayed. Time-history printer plots of pressure, velocity, and temperature at up to 10 user-specified points are generated at run termination. Particle track computations provide the user with particle position history plots for a number of particle sets released at various elapsed times.

2.0 TECHNICAL DESCRIPTION

2.1 Introduction

This section is concerned with the description of a mathematical and computer model for the analysis of coupled thermal and fluid flow in porous media. The mathematical model is based upon the classical equations of porous media flow⁽³⁾ with temperature-dependent water properties. It is suitable for both steady- and unsteady-state flow. The model also allows for anisotropy of hydraulic conductivities and variation of the hydrologic parameters over space and time. In its present form, it is a two-dimensional model and a solution to the governing mathematical equations is obtained by a combination of the alternation-direction-implicit technique with integrated finite differences. The resulting algorithm is numerically stable and possesses an accuracy of the second-order in the space and of the first-order in the time domain. A full discussion of the theoretical basis and the numerical characteristics of such methods is given by Yanenko.⁽⁴⁾

2.2 The Mathematical Basis

The governing equations for the fluid velocity vector and temperature distribution in an anisotropic porous medium, under constraints of negligible convective acceleration in two dimensional flow, may be written as:⁽³⁾

Pressure equation:

$$S \frac{\partial P}{\partial t} = \frac{1}{r} \frac{\partial}{\partial x} (r D_{xx} \frac{\partial P}{\partial x}) + \frac{\partial}{\partial y} (D_{yy} \frac{\partial P}{\partial y}) + \frac{\partial}{\partial y} (D_{yy} R) + S_p \quad (2.2-1)$$

Temperature equation:

$$\begin{aligned} C_c \frac{\partial T}{\partial t} = & - \frac{1}{r} \frac{\partial}{\partial x} (r C_f u T) - \frac{\partial}{\partial y} C_f v T + \frac{T}{r} \frac{\partial}{\partial x} r C_f u \\ & + T \frac{\partial}{\partial y} C_f v + \frac{1}{r} \frac{\partial}{\partial x} (r \Gamma \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (\Gamma \frac{\partial T}{\partial y}) \\ & + S_o - C_f S_p T \end{aligned} \quad (2.2-2)$$

where:

- C_c is the heat capacity per unit volume
- C_f is the heat capacity of the fluid per unit volume
- D_{xx} is the hydraulic conductivity in the x direction
- D_{yy} is the hydraulic conductivity in the y direction
- g is the coefficient of gravitational acceleration
- P is the total pressure defined as $P/\rho_0 g + y$
- r is the radial coordinate
if $r = 1$ the equations above are given in the cartesian coordinate system
- $r = x$ the equations above are given in the cylindrical coordinate system
- S is the specific storativity
- S_o is the heat source per unit volume per unit time
- S_p is the fluid input per unit volume per unit time
- T is the temperature
- t is the time coordinate
- u is the velocity component in the x direction
- v is the velocity component in the y direction
- x is the horizontal coordinate

y is the vertical coordinate

Γ is the thermal conductivity

ρ_0 is the reference value of density

The parameters D_{xx} and D_{yy} are defined as:

$$D_{xx} = K_{xx} / M$$

$$D_{yy} = K_{yy} / M \quad \text{.....(2.2-3)}$$

where $K_{xx} = k_{xx} \rho_0 g / \mu_0$

$$K_{yy} = k_{yy} \rho_0 g / \mu_0 \quad \text{.....(2.2-4)}$$

$$M = \mu / \mu_0 \quad \text{.....(2.2-5)}$$

K_{xx} and K_{yy} are the terms on the diagonal of the anisotropic reference hydraulic conductivity tensor, k_{xx} and k_{yy} are the corresponding components of the intrinsic permeability tensor, M is the viscosity ratio parameter, and μ_0 is the reference value of the viscosity μ .

The pressure and temperature fields $P(x,y,t)$, $T(x,y,t)$ are computed by solving Equations 2.2-1 and 2.2-2. The horizontal and vertical components, denoted respectively by u and v are then computed by:

$$u = - D_{xx} \frac{\partial P}{\partial x}$$

$$v = - D_{yy} \left[\frac{\partial P}{\partial y} + R \right] \quad \text{.....(2.2-6)}$$

where R is the density deficit parameter defined as $R = \rho / \rho_0 - 1$ (2.2-7)

With σ as the effective porosity of the porous medium, the fluid particle velocities are given by:

$$U = u / \sigma, \quad V = v / \sigma. \quad \text{.....(2.2-8)}$$

For the steady-state flow, a stream function, ψ , can be defined so as to satisfy the continuity equation identically. In terms of the velocity components, it is given by:

$$ru = \partial\psi/\partial y, \quad rv = -\partial\psi/\partial x \quad (2.2-9)$$

Or:

$$\begin{aligned} \psi &= \psi_0 + \int_{y_0}^y rudy, \text{ along constant } x, \text{ and} \\ \psi &= \psi_0 - \int_{x_0}^x rvdxdx, \text{ along constant } y, \end{aligned} \quad (2.2-10)$$

where (x_0, y_0) is an arbitrary reference point and ψ_0 is the arbitrary reference value of the stream function.

From Equation 2.2-10 it is easily seen that the stream function or rather the difference between the stream function values at two points is representative of the volumetric flow (per unit length normal to the x, y plane for Cartesian coordinates) between the two points of the flow. Further, it can be shown⁽³⁾ that, for steady-state flow, lines of constant stream function, called streamlines, are identical with the fluid path or flow lines. Thus, on balance, no fluid particles flow across any given streamlines.

2.3 The Water Properties

For the applications of concern, the water properties, the density ρ and the viscosity μ , are considered to be a primary function of temperature alone. In general, the effects of temperature and pressure should both be accounted for. However, typically the variations of ρ and μ are much stronger functions of temperature than of pressure.

A recommended relation for extrapolation of water density ρ , from a known value ρ_0 at a temperature T_0 , to a temperature T below the critical temperature T_c is ⁽⁵⁾:

$$\rho = \rho_0 \left[(T_c - T) / (T_c - T_0) \right]^\alpha \quad (2.3-1)$$

The density deficit parameter R of Equation 2.2-7 is then given by:

$$R = \rho / \rho_0 - 1 = (T_c - T)^\alpha (T_c - T_0)^{-\alpha} - 1 \quad (2.3-2)$$

For the range of concern the best fit of the calculated values with the tabulated values was obtained with α equal to 0.20. The critical temperature for water is 647.3°K or 705.47°F.

The effect of temperature on the viscosity of a liquid may be correlated with the de Guzman-Andrade equation ⁽⁵⁾ by:

$$\mu = A \exp (B/T) \quad (2.3-3)$$

where A and B are constants and the temperature T is in absolute units.

The viscosity-ratio parameter M of Equation 2.2-5, is then written as:

$$M = \nu / \nu_0 = \exp (B/T - B/T_0) \quad (2.3-4)$$

For the range of concern a value of B equal to 1436°K or 2584.8°R was selected to provide good agreement with the available tabulated data.

2.4 The Numerical Method

The porous media flow Equation 2.2-1 and the temperature distribution Equation 2.2-2 were incorporated in a computer model called GWTHERM to signify Ground Water flow with THERMal gradients. The method of solution adopted was a combination of the well-established Alternating Direction Implicit technique (ADI) with an Integrated Finite Differences technique (IFD).

Consider the finite difference grid and the grid cell shown in Figure 2.4-1. In the ADI technique, from the known solution at time t^n ,

$$RP(I) = (RU(I) + RU(I+1))/2.$$

FIGURE 2.4-1

GRID CELL

PROGRAM NOTATION	MATHEMATICAL NOTATION
$X(I)$	x_i
$Y(J)$	y_j
$XU(I)$	$\frac{1}{2}(x_i + x_{i-1})$
$YV(J)$	$\frac{1}{2}(y_j + y_{j-1})$
$DX(I)$	δx_i
$DY(J)$	δy_j
$DXM(I)$	$x_i - x_{i-1}$
$DYM(J)$	$y_j - y_{j-1}$
$U(IJ)$	u_{ij}
$V(IJ)$	v_{ij}
$P(IJ)$	p_{ij}
$GAMX(IJ)$	$K_{xx_{ij}}$
$GAMY(IJ)$	$K_{yy_{ij}}$
$TEMP(IJ)$	T_{ij}
$GMU(IJ)$	M_{ij}
$RHO(IJ)$	R_{ij}
$RGD(IJ)$	ψ_{ij}
$RU(I)$	$r_{\frac{1}{2}-i}$
$TGAM(IJ)$	Γ_{ij}
$TCC(IJ)$	$n C_f \rho_f + (1-n) \rho_s C_s$
$TCF(IJ)$	$\rho_f C_{f_{ij}}$

the solution at time t^{n+1} is obtained in two steps. In the first, a discrete approximation to 2.2-1 and 2.2-2 is obtained from:

$$2S (P_{ij}^{n+\frac{1}{2}} - P_{ij}^n) = \delta t (F_x^{n+\frac{1}{2}} + F_y^n) \quad (2.4-1)$$

and
$$2C_c (T_{ij}^{n+\frac{1}{2}} - T_{ij}^n) = \delta t (G_x^{n+\frac{1}{2}} + G_y^n) \quad (2.4-2)$$

where F_x , F_y , G_x and G_y are the x and y directional components of the differential operator on the right hand side of Equations 2.2-1 and 2.2-2. respectively.

The time step is completed with a second half-step obtained from:

$$2S (P_{ij}^{n+1} - P_{ij}^{n+\frac{1}{2}}) = \delta t (F_x^{n+\frac{1}{2}} + F_y^{n+1}) \quad (2.4-3)$$

and
$$2C_c (T_{ij}^{n+1} - T_{ij}^{n+\frac{1}{2}}) = \delta t (G_x^{n+\frac{1}{2}} + G_y^{n+1}) \quad (2.4-4)$$

2.4.1 First Half-Step Pressure Equation

During the first half-step, Equation 2.4-1 leads to the algebraic analogue:

$$A_i P_{i+1,j}^{n+\frac{1}{2}} + B_i P_{i-1,j}^{n+\frac{1}{2}} + C_i = D_i P_{ij}^{n+\frac{1}{2}} \quad (2.4-5)$$

where

$$A_i = (D_{xx})_{i+\frac{1}{2},j} r_{i+\frac{1}{2}} / (x_{i+1} - x_i)$$

$$B_i = A_{i-1}$$

$$C_i = \frac{S \delta x_i r_i}{\frac{1}{2} \delta t} P_{ij}^n + (v_{ij}^n - v_{i,j+1}^n) \frac{\delta x_i}{\delta y_j} r_i + S_{p_{ij}} \delta x_i r_i$$

$$D_i = \frac{S \delta x_i r_i}{\frac{1}{2} \delta t} - A_i - B_i \quad (2.4-6)$$

2.4.2 First Half-Step Temperature Equation

The algebraic analogue to Equation 2.4-2 at the first half of the time step is:

$$A_i T_{i+1,j}^{n+\frac{1}{2}} + B_i T_{i-1,j}^{n+\frac{1}{2}} + C_i = D_i T_{i,j}^{n+\frac{1}{2}} \quad (2.4-7)$$

where

$$\begin{aligned} A_i &= -b_e + \frac{1}{2} c_e u_e^{n+\frac{1}{2}} (1 - \alpha_e) \\ B_i &= -b_w - \frac{1}{2} c_w u_w^{n+\frac{1}{2}} (1 + \alpha_w) \\ C_i &= c_p T_p^n + (T_n^n - T_p^n) \left[b_n - \frac{1}{2} c_n v_n^n (1 - \alpha_n) \right] \\ &\quad + (T_s^n - T_p^n) \left[b_s + \frac{1}{2} c_s v_s^n (1 + \alpha_s) \right] \\ &\quad + S_o \delta x_i \delta y_j r_i \\ D_i &= c - A_i - B_i + S_p c_{fp} \delta x_i \delta y_j r_p \end{aligned} \quad (2.4-8)$$

The parameter α in 2.4-8 is defined:

$\alpha_{e,w} = 0$ if $ u < \sigma_{e,w}$	$\alpha_{n,s} = 0$ if $ v < \sigma_{n,s}$
$\alpha_{e,w} = 1$ if $u > \sigma_{e,w}$	$\alpha_{n,s} = 1$ if $v > \sigma_{n,s}$
$\alpha_{e,w} = -1$ if $-u > \sigma_{e,w}$	$\alpha_{n,s} = -1$ if $-v > \sigma_{n,s}$

$$\begin{aligned} \sigma_{e,w} &= \frac{2\Gamma_{e,w}}{\delta x_{e,w} c_{fe,w}} \\ \sigma_{n,s} &= \frac{2\Gamma_{n,s}}{\delta y_{n,s} c_{fn,s}} \end{aligned} \quad (2.4-9)$$

The coefficients b , c , and c_p in 2.4-8 are defined as:

$$c_p = \frac{\delta x \delta y r_p C_c}{\delta t / 2} \quad (2.4-10)$$

$$\begin{aligned} b_e &= \frac{\delta y r_e \Gamma_e}{\delta x_e} = \frac{\delta y r_e (\Gamma_E + \Gamma_p)}{2 \delta x_e} \\ b_w &= \frac{\delta y r_w \Gamma_w}{\delta x_w} = \frac{\delta y r_w (\Gamma_W + \Gamma_p)}{2 \delta x_w} \\ b_n &= \frac{\delta x r_p \Gamma_n}{\delta y_n} = \frac{\delta x r_p (\Gamma_N + \Gamma_p)}{2 \delta y_n} \\ b_s &= \frac{\delta x r_p \Gamma_s}{\delta y_s} = \frac{\delta x r_p (\Gamma_S + \Gamma_p)}{2 \delta y_s} \end{aligned} \quad (2.4-11)$$

$$\begin{aligned} \frac{1}{2} c_e &= \frac{1}{2} r_e \delta y C_{fe} \\ &= \frac{1}{4} r_e \delta y (C_{fE} + C_{fp}) \end{aligned}$$

$$\begin{aligned} \frac{1}{2} c_w &= \frac{1}{2} r_w \delta y C_{fw} \\ &= \frac{1}{4} r_w \delta y (C_{fW} + C_{fp}) \end{aligned}$$

$$\begin{aligned} \frac{1}{2} c_n &= \frac{1}{2} r_n \delta x C_{fn} \\ &= \frac{1}{4} r_p \delta x (C_{fN} + C_{fp}) \end{aligned}$$

$$\begin{aligned} \frac{1}{2} c_s &= \frac{1}{2} r_s \delta x C_{fs} \\ &= \frac{1}{4} r_p \delta x (C_{fS} + C_{fp}) \end{aligned} \quad (2.4-12)$$

where the subscript convention is:

$$\begin{array}{ll}
 e &= i + \frac{1}{2}, j & E &= i + 1, j \\
 w &= i - \frac{1}{2}, j & W &= i - 1, j \\
 n &= i, j + \frac{1}{2} & N &= i, j + 1 \\
 s &= i, j - \frac{1}{2} & S &= i, j - 1 \\
 & & P &= i, j
 \end{array} \quad (2.4-13)$$

2.4.3 Second Half-Step Pressure Equation

During the second half step Equation 2.4-3 leads to the algebraic analogue:

$$A_j P_{i,j+1}^{n+1} + B_j P_{i,j-1}^{n+1} + C_j = D_j P_{ij}^{n+1} \quad (2.4-14)$$

with

$$A_j = (D_{yy})_{i,j+\frac{1}{2}} / (y_{j+1} - y_j)$$

$$B_j = A_{j-1}$$

$$C_j = \frac{S \delta y_j}{\frac{1}{2} \delta t} P_{ij}^{n+\frac{1}{2}} + \frac{\delta y_j}{\delta x_i r_i} (r_{i-\frac{1}{2},j} u_{i-\frac{1}{2},j} - r_{i+\frac{1}{2},j} u_{i+\frac{1}{2},j})$$

$$+ S p_{ij} \delta y_j + (D_{yy} R)_{i,j+\frac{1}{2}} - (D_{yy} R)_{i,j-\frac{1}{2}}$$

$$D_j = -A_j - B_j + \frac{S \delta y_j}{\frac{1}{2} \delta t} \quad (2.4-15)$$

2.4.4 Second Half-Step Temperature Equation

Equation 2.4-4 leads to the algebraic analogue:

$$A_j T_{i,j+1}^{n+1} + B_j T_{i,j-1}^{n+1} + C_j = D_j T_{ij}^{n+1} \quad (2.4-16)$$

where

$$\begin{aligned} A_j &= -b_n + \frac{1}{2} c_n v_n^{n+1} (1 - \alpha_n) \\ B_j &= -b_s - \frac{1}{2} c_s v_s^{n+1} (1 + \alpha_s) \\ C_j &= c_p T_p^{n+1/2} + (T_E - T_p) \left[b_{e-1/2} c_e u_e^{n+1/2} (1 - \alpha_e) \right] \\ &\quad + (T_W - T_p) \left[b_{w-1/2} c_w u_w^{n+1/2} (1 + \alpha_w) \right] \\ &\quad + S_o \delta x_i \delta y_j r_i \\ D_j &= c_p - A_j - B_j + S_p \delta x_i \delta y_j r_p c_{fp} \end{aligned} \quad (2.4-17)$$

The subscript notation e, w, n, s, E, W, N, S, P and the parameter definition for c_p , b, c are the same as in the first half-step and given in Equations 2.4-10 - 2.4-13.

In each time step the sequence of the main calculation is as follows:

- (1) The first half-time-step pressure equation is solved giving the result of $P^{n+1/2}$;
- (2) u-velocity as a result of $P^{n+1/2}$ is calculated;
- (3) The first half-time-step temperature equation is solved resulting in $T^{n+1/2}$;

- (4) Water properties as a function of $T^{n+\frac{1}{2}}$ are calculated;
- (5) The second half-time-step pressure equation is computed resulting in P^{n+1} ;
- (6) v-Velocity as a result of P^{n+1} is calculated;
- (7) The second half-time-step temperature equation is computed to give T^{n+1} ;
- (8) Water properties as a function of T^{n+1} are calculated.

At each half-step the Equations 2.4-5, 2.4-7, 2.4-14 and 2.4-16 are solved with an efficient tri-diagonal matrix inversion algorithm.

The velocity components, u and v , are obtained from their corresponding differential Equation 2.2-6. In finite-difference notation:

$$u_{ij} = -(D_{xx})_{i-\frac{1}{2},j} (P_{ij} - P_{i-1,j}) / (x_i - x_{i-1}),$$

$$v_{ij} = -(D_{yy})_{i,j-\frac{1}{2}} (P_{ij} - P_{i,j-1}) / (y_j - y_{j-1}) - (D_{yy} R)_{i,j-\frac{1}{2}}$$

(2.4-18)

The fluid particle velocities and the stream function are calculated from the velocity field with difference analogues of Equations 2.2-8 and 2.2-10, respectively.

2.5 Verification:

The computer program, GWTHERM, was verified for a number of test problems to ensure the accuracy of the algorithm and proper working of the program logic. All of the test problems selected were such that analytical solutions were available for purposes of comparison with the numerical solutions obtained by GWTHERM.

2.5.1 Test Case 1

One dimensional linear temperature distribution

Given a pressure field $P = P_0 + P_1 xy$ (2.5-1)
 where P_0 and P_1 are arbitrary constants, the velocity field under conditions of uniform water properties is given by:

$$\begin{aligned} v &= 0 \\ u &= Ay \end{aligned} \quad (2.5-2)$$

Holding the temperature at $x = 0$ equal to T_0
 and at $x = \ell$ equal to T_ℓ

the temperature field is

$$T = T_0 + \frac{T_\ell - T_0}{\ell} x \quad (2.5-3)$$

This problem was numerically solved by the program on a unit square and the results appeared to be identical with the analytical solution 2.5-3 up to at least 4 significant digits.

2.5.2 Test Case 2

Temperature distributions in a uniform velocity field

Given the velocity field

$$\begin{aligned} v &= 0 \\ u &= u_0 \end{aligned} \quad (2.5-4)$$

and holding the temperature at the boundaries constant:

$$\begin{aligned} T(0, y) &= T_0 \\ T(\ell, y) &= T_\ell \end{aligned} \quad (2.5-5)$$

The temperature distribution for this case is given:

$$T = (T_o e^u - T_\ell) / (e^u - 1) + [(T_\ell - T_o) / (e^u - 1)] \exp\left(\frac{u x}{\ell}\right) \quad (2.5-6)$$

The problem was solved on a unit square ($0 \leq x \leq 1$), ($0 \leq y \leq 1$) with the following input:

$$\begin{aligned} T(0, y) &= 20 \\ T(1, y) &= 37.18 \\ v &= 0 \\ u &= 1 \end{aligned} \quad (2.5-7)$$

A grid spacing of 0.05 was selected.

As the steady-state is reached asymptotically the computer simulation was therefore carried out up to 0.5 time units in steps of 0.01 units.

The numerical solution so obtained is identical to the analytical solution up to at least 3 significant digits.

2.5.3 Test Case 3

Temperature of fluid in a state of solid body rotation⁽¹⁾

The velocity field is given by:

$$\begin{aligned} u &= 2y \\ v &= -2x \end{aligned} \quad (2.5-8)$$

THE PROBLEM AND THE CONTROL VOLUME

The exact solution for this case is:

$$T = -\frac{1}{2} \frac{1}{r} \log(x^2 + y^2) + \text{constant} \quad (2.5-9)$$

The numerical results were obtained for a square-shaped control volume as shown with half a diagonal of the square equal to unity. The corner nearest to the origin of the co-ordinate system was one unit away from it. The value of r was adjusted to obtain minimum value of zero at the outermost corner and a maximum value of one at the innermost corner.

The control volume was covered by an 11 x 11 grid with uniform spacing.

The initial value of the temperature at all interior grid points was set to zero.

The simulation was carried out for a duration of 0.7 time units in steps of 0.01 units.

The numerical solution and the analytical solution are in excellent agreement.

A sample comparison is given in the table below.

<u>LOCATION</u> (x,y)	<u>TEMPERATURE</u>	
	Analytical	Computed
(0.71, 0.71)	1.00	1.00
(0.849, 0.99)	0.834	0.834
(1.41, 1.41)	0.369	0.369
(1.70, 1.56)	0.241	0.241
(2.12, 2.12)	0.0	0.0

2.5.4 Test Case 4

Modelling of underground storage in an aquifer of hot water⁽²⁾

In this case temperature and water velocity and pressure distributions as a function of time and radial distance from a well are simulated.

This problem has a radial symmetry with the well at the zero radial distance. The aquifer depth (100-200m) is confined by impermeable caprock and bedrock. The top of the caprock and the bottom of the bedrock are kept at a constant temperature of 20°C. The initial temperature of the aquifer is 20°C. Hot water (220°C) is injected at a rate of 10^6 kg/day for a period of 90 days. Then water is pumped out through the well at the same rate for another 90 days.

A numerical solution to this case is also given in Reference 2.

This problem was solved with a similar grid spacing as the one chosen in Reference 2 and with a time step of 3 days.

Sample results of the two models are given below and seem to agree fairly well.

LOCATION (r,y)	TEMPERATURE AFTER 90 DAYS		TEMPERATURE AFTER 180 DAYS	
	Ref 2	GW THERM	Ref 2	GW THERM
0,180	220°C	220°C	>100°C	99.2°C
14,180	220°C	220°C	100°C	69.1°C
34,180	40°C	39.0°C	30°C	21.7°C

Property parameters
used in hot water
storage model.

	Reservoir (Sandstone)	Caprock-Bedrock (Mudstone)
Porosity	0.20	1×10^{-20}
Density kg m^{-3}	2.6×10^3	2.7×10^3
Heat Capacity $\text{J kg}^{-1} \text{ } ^\circ\text{C}^{-1}$	9.70×10^2	9.30×10^2
Thermal Conductivity $\text{J s}^{-1} \text{m}^{-1} \text{ } ^\circ\text{C}^{-1}$	2.894	1.157
Permeability m^2	1×10^{-13}	1×10^{-40}
Specific Storage $\text{N}^{-1} \text{m}^2$	1×10^{-3}	1×10^{-12}

F L U I D P A R A M E T E R S			
Viscosity (cp)	$T(^{\circ}\text{C})$	Heat Capacity ($\text{J kg}^{-1} \text{ } ^\circ\text{C}^{-1}$)	$T(^{\circ}\text{C})$
1.005	20	4.127×10^3	25
5.45×10^{-1}	50	3.894×10^3	75
2.80×10^{-1}	100	3.652×10^3	125
1.82×10^{-1}	150	3.341×10^3	200
1.35×10^{-1}	200		
Expansivity ($^{\circ}\text{C}^{-1}$) 3.17×10^{-4}			

2.5.5 Test Case 5

Temperature distribution in a ring

This example illustrates the use of cylindrical coordinates

A ring of conductive material is kept at a constant temperature in its inner and outer radii.

$$\begin{aligned} T(r_{in}) &= T_1 \\ T(r_{out}) &= T_2 \end{aligned} \tag{2.5-10}$$

The temperature distribution for this case is

$$T = A \log(r) + \text{constant} \tag{2.5-11}$$

This problem was solved numerically for a ring

$$\begin{aligned} r_{in} &= 0.4 & r_{out} &= 1.0 \\ \text{with } T_{in} &= 0.08 & T_{out} &= 1.0 \end{aligned}$$

The initial temperature was chosen to be zero.

The solution was carried out to a duration of 0.5 time units with a time interval of 0.02 units where a steady-state was reached.

The numerical solution and the analytical solution agree very well as can be seen from the table below.

r	TEMPERATURE	
	Analytic	Computed
0.4	0.0837	0.0837
0.5	0.307	0.307
0.7	0.643	0.643
0.9	0.895	0.894
1.0	1.00	1.00

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APPENDIX 6

ADDITIONAL RESULTS FROM COUPLED HEAT
AND GROUNDWATER FLOW

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 100 YEARS

FIGURE 1

TRACKS OF PARTICLES RELEASED AT 100 YEARS, CASE I

HANFORD HLW REPOSITORY 25W/M2

TEMPERATURE PLOT

TIME = 100 YEARS

FIGURE 2

TEMPERATURE CONTOURS AT 100 YEARS, CASE I

YANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 100 YEARS

FIGURE 3

GROUNDWATER FLOW VELOCITIES AT 100 YEARS, CASE 1

HANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 100 YEARS

FIGURE 4

GROUNDWATER FLOW VELOCITIES AT 100 YEARS, CASE 1

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 1000 YEARS
DISTANCE (km)

FIGURE 5

TRACKS OF PARTICLES RELEASED AT 1000 YEARS, CASE 1

HANFORD HLW REPOSITORY 25W/M2

TEMPERATURE PLOT

TIME = 1000 YEARS

DISTANCE

0

10km

FIGURE 6

TEMPERATURE CONTOURS AT 1000 YEARS, CASE 1

HANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 1000 YEARS

SCALE = 7 HORIZONTAL AND 1 VERTICAL

FIGURE 7

GROUNDWATER FLOW VELOCITIES AT 1000 YEARS, CASE 1

HANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 1000 YEARS

FIGURE 8

GROUNDWATER FLOW VELOCITIES AT 1000 YEARS, CASE 1

299
HANFORD HLW REPOSITORY

RHO-BWI-C-23
25W/M2

TEMPERATURE PLOT

TIME = 10000 YEARS

FIGURE 9

TEMPERATURE CONTOURS AT 10,000 YEARS, CASE 1

HANFORD HLW REPOSITORY

25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 10000 YEARS

FIGURE 10

GROUNDWATER FLOW VELOCITIES AT 10,000 YEARS, CASE 1

HANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 10000 YEARS

FIGURE 11

GROUNDWATER FLOW VELOCITIES AT 10,000 YEARS, CASE 1

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 100 YEARS
DISTANCE (km)

FIGURE 12

TRACKS OF PARTICLES RELEASED AT 100 YEARS, CASE 2

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 1000 YEARS
DISTANCE (km)

FIGURE 13

TRACKS OF PARTICLES RELEASED AT 1000 YEARS, CASE 2