APPLICATION OF GEOTHER/VT4 TO ASSESS GROUNDWATER TRANSIENTS IN A HIGH LEVEL RADIOACTIVE WASTE REPOSITORY

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ABSTRACT

The GEOTHER/VT4 computer code is an improved version of the GEOTHER computer code. The GEOTHER/VT4 code was applied to a two-dimensional simulation of a waste package in a high-level waste repository to predict the thermal-hydraulic environment where steam formation may occur. The thermal-hydraulic environment is important for assessing waste package container corrosion and packing material swelling behaviors, and evaluation of the near-field geochemical conditions. The waste package was assumed to be situated in the Cohassett flow of the Hanford Site, located in Washington State. This analysis provides the first assessment of the duration and size of a two-phase environment for the waste package.

1.0 INTRODUCTION

The GEOTHER/VT4 code has been developed at the Pacific Northwest Laboratory (PNL) in support of Basalt Waste Isolation Project (BWIP) effort. This code is based on the GEOTHER code (Faust and Mercer 1983) but has been improved to make it suitable for the high-level radioactive waste repository applications. The objective of this work is to assess thermal-hydraulic conditions resulting from nuclear heating effects in the high-level radioactive waste package and its surroundings where a two-phase (steam and water) condition may occur.

The waste package is an engineered barrier used to isolate high-level radioactive waste from the accessible environment. The current BWIP waste package design (see Fig. 1) consists of the radioactive waste, a container, and packing material. The groundwater and thermal conditions provide decision-making information for waste package container corrosion and packing material swelling testing program, and evaluation of the near-field geochemical conditions.

2.0 THE GEOTHER/VT4 CODE

The GEOTHER/VT4 code is a three-dimensional, two-phase groundwater simulation code. The code is based on a general mathematical model of a waste repository system that describes the three-dimensional flow of groundwater (vapor and liquid water) and heat transport from nuclear waste in a porous medium. The code solves the mass, momentum, and energy balance equations for vapor and liquid water and a heat conduction equation for porous/nonporous materials (e.g., host rock and waste container).

Using Darcy's Law in place of the momentum equations, the conservation equations are reduced to three nonlinear partial differential equations in terms of the dependent variables, pressure, enthalpy, and rock/solid temperature.

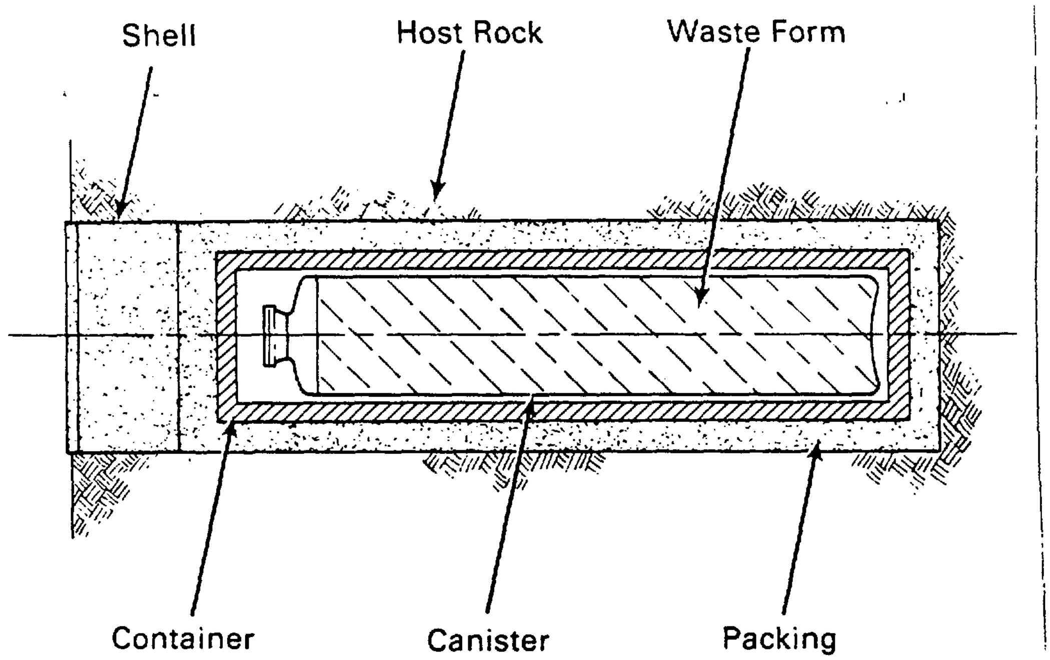

FIGURE 1. BWIP Waste Package Design

The mass balance is calculated as follows:

$$\frac{\partial(\phi\rho)}{\partial t} - \nabla\cdot\left[\frac{kK_{rs}\rho_s}{\mu_s}(\nabla p - \rho_s g\nabla D)\right] - \nabla\cdot\left[\frac{kK_{rw}\rho_w}{\mu_w}(\nabla p - \rho_w g\nabla D)\right] - q'_m = 0 \qquad (1)$$

The water energy balance equation is as follows:

$$\frac{\partial}{\partial t}(\phi\rho h) - \nabla\cdot\left[\frac{kK_{rs}\rho_s h_s}{\mu_s}(\nabla p - \rho_s g\nabla D)\right] - \nabla\cdot\left[\frac{kK_{rw}\rho_w h_w}{\mu_w}(\nabla p - \rho_w g\nabla D)\right]$$

$$- \nabla\cdot\left[K_m\left(\frac{\partial T}{\partial p}\right)_h\nabla p + K_m\left(\frac{\partial T}{\partial h}\right)_p\nabla h\right] - q'_{h_{sw}} - h_{rw}(T_r - T) = 0 \qquad (2)$$

The rock/solid energy balance equation is set up as follows:

$$\frac{\partial}{\partial T}\left[(1-\Phi)\rho_r C_r T_r\right] - \nabla\cdot K_r\nabla T_r - q'_{h_r} + h_{rw}(T_r - T) = 0 \qquad (3)$$

where

∇ = the vector differential operator
t = time
ϕ = porosity
k = the intrinsic permeability tensor of the porous medium

K_{rs} = the relative permeability of steam phase
ρ_s = the steam density
μ = the dynamic viscosity
p = pressure
g = the gravitational acceleration
D = the depth
K_{rw} = the relative permeability of water phase
w = the liquid water
ρ_w = the water density
q_m' = source term for mass
ρ = the steam-water mixture density
h = the enthalpy of two-phase mixture
K_m = the medium conduction-dispersion coefficient
T = the steam/water temperature
$q_{h_{sw}}'$ = the source term for water energy
h_{rw}^{sw} = the heat conductance between rock and water
T_r = the rock/solid temperature
ρ_r = the rock density
C_r = the rock specific heat
K_r = the rock thermal conductivity
q_{h_r}' = the heat input to rock by external heat sources such as nuclear waste decay heat
$_s$ = the steam
$_r$ = the rock/solid

In the code, C_r and K_r are considered functions of rock/solid temperatures. The relative permeability (K_{rs} or K_{rw}) is a factor used to account for the relative velocities between the steam and water phases. Relative permeability is a function of the saturation values of each phase. Two functional forms for K_{rs} and K_{rw} are available in the GEOTHER/VT4 code. One is the linear form and the other is the Corey correlation (Bear 1972).

The water thermodynamic properties functions are adapted from the Electric Power Research Institute (EPRI) algorithms (Stewart et al. 1983). The functions are valid for pressures ranging from 700 to 4 x 10^7 Pa and specific enthalpies ranging from approximately 5 x 10^5 to 4 x 10^6 J/kg.

The numerical techniques used in the GEOTHER/VT4 code to solve equations 1, 2, and 3 are the same techniques used by Faust and Mercer (1983).

2.1 Boundary Conditions

Equations 1, 2, and 3 comprise a set of nonlinear second-order partial-differential equations. Three boundary conditions (pressure, enthalpy, and rock temperature) are required at the boundaries. Two types of boundary conditions are currently available in the code. The first is a zero-flux type, which indicates a no-flow boundary for both mass and heat. The second condition is a constant parameter type where water pressure, enthalpy, and rock temperature are fixed at the boundary.

2.2 Assumptions and Limitations in the Code

The major assumptions made in the mathematical formulations are as follows:

1. Flow is through a porous medium where Darcy's law is valid.
2. Capillary pressure effects are negligible.

3. The system is single-component water consisting of either one or two phases. Thermal equilibrium exists between the steam and water.
4. Relative permeability is a function of liquid volume saturation; hysteresis is neglected.
5. Rock enthalpy is a linear function of temperature.
6. Kinetic, potential energy, and compression work are negligible.
7. Thermal conductivity is combined for a steam and water mixture. It is a constant, isotropic lumped parameter that represents both conduction and thermal dispersion.

3.0 TWO-DIMENSIONAL WASTE PACKAGE SIMULATION

The GEOTHER/VT4 code has been applied to a two-dimensional simulation of a waste package container in the basalt repository environment. In this simulation, the waste packages are assumed to be situated in the Cohassett flow of the BWIP site bounded by the flow top and flow bottom. The pressures are assumed to be invariant at the flow top and bottom after the waste package emplacement. By assuming that all waste packages are the same and by invoking the geometric symmetry, a cut-through section with a single waste package is used to represent a typical waste package condition in the basalt repository. Because of the two-dimensional simplification, the containers are modeled as heat slabs.

Figure 2 shows the model's front view with dimensions. The waste package container and packing are emplaced at the same time. The placement room is kept open to the atmosphere for 50 years before backfill. The region where the waste package is located is simulated using the heat conduction equation (Eq. 3). The fluid into and out of the container is set to zero. All other regions are simulated with Equations 1, 2 and 3. A best-estimate case is presented here. The heat generation rate is reduced from the actual value of 2.1 kW per container to about 0.6 kW per container so that the maximum container temperature matches that from a three-dimensional calculation using the conduction code HEATING5 (Yung et al. 1985). This modification is necessary because of the two-dimensional approximation of a three-dimensional model. (The containers are assumed to be next to each other, side-by-side, whereas in actual design they are 6.7 m apart.)

Figure 3 shows the representative results of two-phase formation surrounding the waste package container. The contours define the two-phase region. The region inside the contour is the two-phase mixture; the region outside the contour is subcooled liquid. After the waste package is emplaced, it heats up the packing material and the surrounding host rock and steam starts to form. This occurs shortly after waste package emplacement. At 1.3 years (Fig. 3), the container is partially surrounded by two-phase saturated (in a thermodynamice sense)[a] water (i.e., the packing next to the container in the borehole is partially filled with steam).

As the heat-up process continues, the contour expands gradually. When the two-phase zone is approaching its maximum, it extends about 0.5 m above and below the container surface. As the heat generation rate and the heat loss rate become about equal in the near field, the saturation

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(a) Saturation has two definitions: 1) without specification saturation means the liquid water volume fraction in a two-phase water and steam system, and 2) saturation means thermodynamic saturation (e.g., saturation line in a pressure and enthalpy diagram).

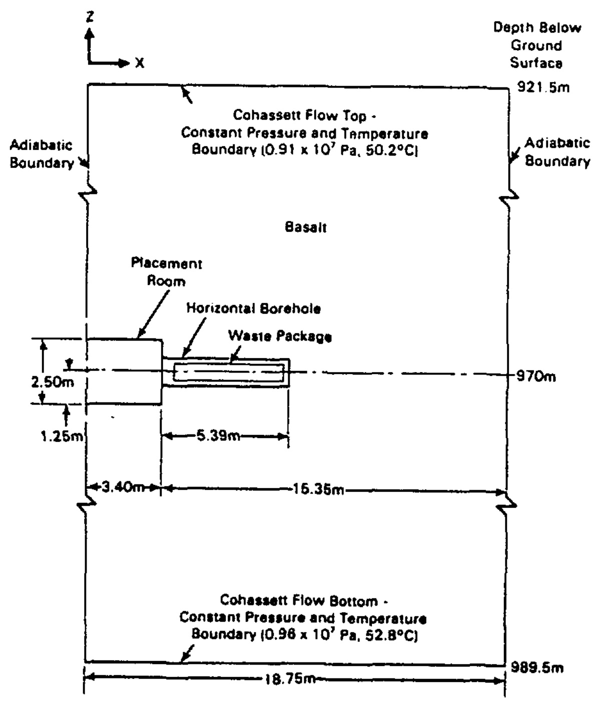

FIGURE 2. Detailed XZ Plane Dimensions of the Two-Dimensional Cartesian Model

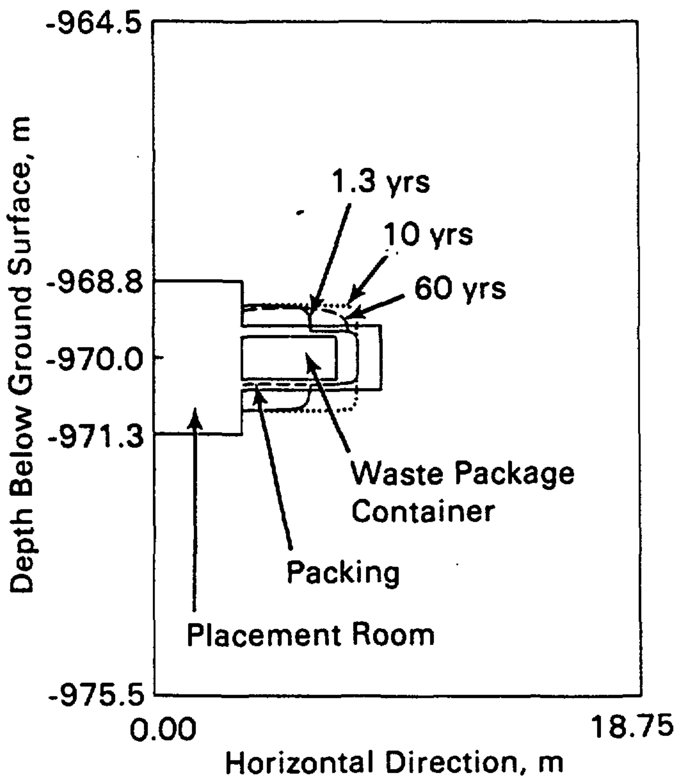

FIGURE 3. Contour of Groundwater Saturation

profile stabilizes. This happens from 10 to 50 years after container emplacement. At 50 years, the placement room is backfilled. The loss of pressure sink (i.e., the open placement room) causes the near-field pressure to increase rapidly. This leads to a rapid decrease of the two-phase zone right after the placement room closure.

As the transient proceeds, the rate of decrease becomes slower. This is due to the slower rate of decrease of decay heat, continued heat loss to the boundary, and influx of liquid groundwater. The contour plot at 60 years after container emplacement is given in Fig. 3. After this, the steam in the two-phase zone is totally condensed and the near field is resaturated at about 62 years. Figure 4 gives the velocities of the liquid groundwater at 1.3 years after the container emplacement. The flow is toward the container and the placement room. This inward flow is caused by the pressure gradients from the higher pressures at the flow top and bottom and the lower pressure at the placement room.

Figure 5 gives the groundwater flow at the time of resaturation. By looking at the groundwater flow directions, the pressures near the container stay below the boundary pressures even after the placement room is backfilled (50 years after container emplacement). This is because at the time of closure, the pressure is 1 atm in the placement room. Even though the backfill results in the loss of pressure sink, the pressure in the near field does not increase significantly. This is due to the very limited amount of groundwater influx toward the container (low permeabilities) and the larger amount of heat loss to the host rock through conduction. After the near field is resaturated (62 years), the pressure begins

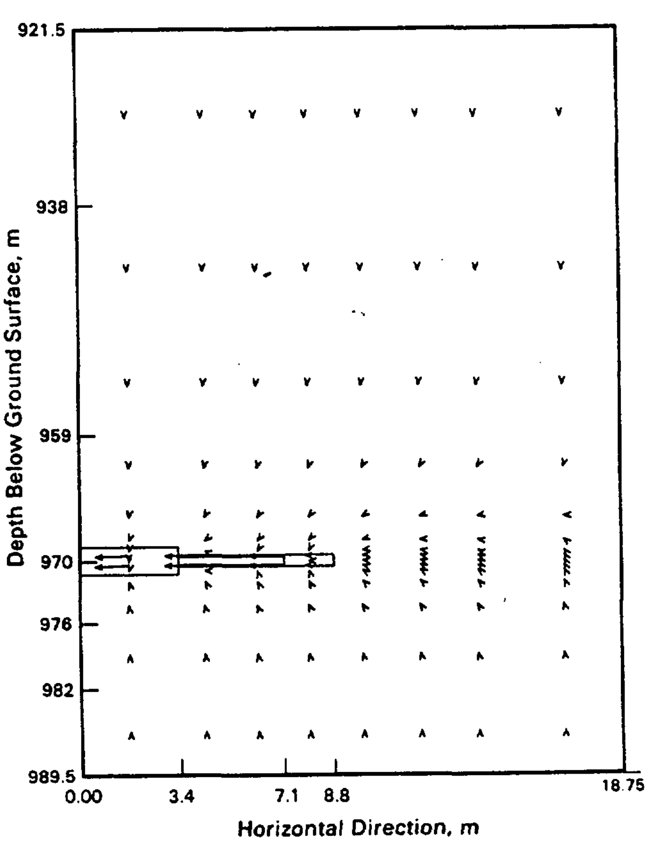

FIGURE 4. Velocity Vectors, 1.3 Years after Waste Package Emplacement

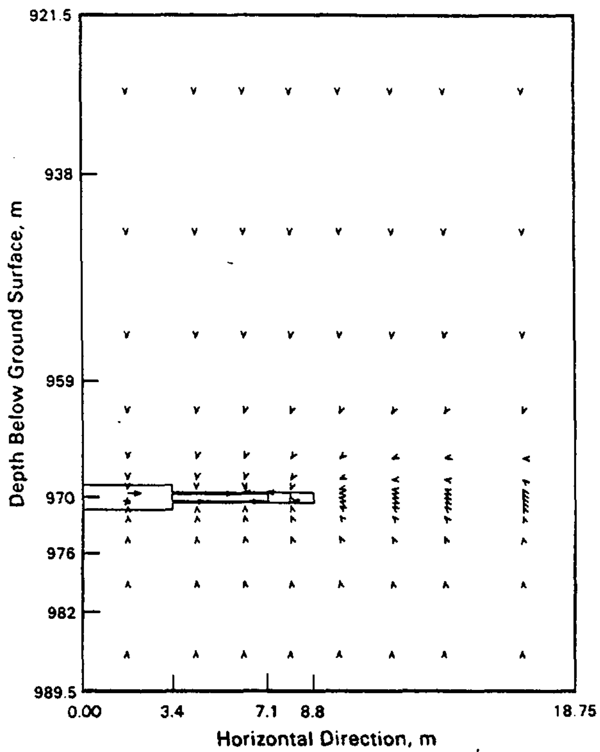

FIGURE 5. Velocity Vectors, 60 Years after Waste Package Emplacement

to increase gradually because of the continued heat generation input and the influx of the groundwater. The rate of increase is very slow because of the low permeability. At the end of simulation (1,000 years), the pressure in the backfill region is about 0.6% lower than the unperturbed hydrostatic pressure. So the system essentially returns to the unperturbed state.

Figure 6 is a plot of the container temperature (volume averaged). This temperature was calculated by the conduction equation (Eq. 3) added to the code. The container is at an ambient temperature of 52°C at the time of emplacement (Fig. 6). It goes through a rapid heatup after borehole backfill because of the much slower heat loss through the backfill and host rock than through the 52°C temperature sink. A maximum of ~220°C occurs around 3 years after container emplacement. After that, the decay heat generation rate becomes less than the heat loss rate immediately adjacent to the container. At this point, the container temperature starts to decrease gradually. At the time of placement room backfilling, the container temperature increases due to the loss of the 52°C temperature sink in the placement room. After this increase, the decay heat drops and the container temperature starts to decrease again as the heat loss to boundary becomes larger than the decay heat. At 1,000 years, the temperature drops to 70°C.

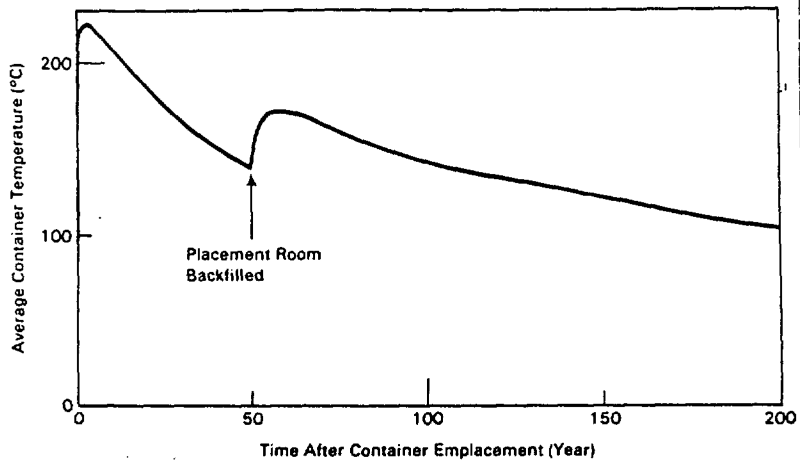

FIGURE 6. Container Temperature Versus Time

4.0 SUMMARY

The need for a realistic simulation of the geothermal conditions in a high-level radioactive waste repository led to the development of the GEOTHER/VT4 code. This code is a modification of the GEOTHER code to allow simulation of waste packages, the continuous changing heat generation source, the expansion of water thermodynamic property ranges.

From a simplified two-dimensional model with a best-estimate heat generation rate, the code predicts that the two-phase mixture forms in the region next to the container almost immediately after the emplacement. About 10 years after emplacement, the two-phase zone reaches its maximum size, about 0.5 m above and below the container surface. After this period, the saturation profile stays essentially unchanged until 50 years after container emplacement, when the placement room is backfilled. After that, the two-phase zone starts to condense due to a short period of pressure increase and a long-term gradual decrease of decay heat and influx of liquid groundwater. The near field is totally resaturated 62 years after container emplacement.

This analysis provided the first estimation of the duration and size of the two-phase region of a high-level radioactive waste repository in basalt. This information is important in determining waste container and packing material testing programs.

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