NUMERICAL MODELING OF RADIONUCLIDE TRANSPORT THROUGH REPOSITORY SEALS

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ABSTRACT

The mathematical basis of a two-dimensional model for estimating transport of radionuclides through repository seals for an underground nuclear waste repository is described. The model consists of three coupled equations, one each for fluid flow, heat transfer, and mass transport. Thus, the model includes transport of radionuclides due to convection (induced by natural hydraulic gradients and by density differences created by radiogenic heat), hydrodynamic dispersion, and molecular diffusion. A short summary of the numerical procedure used to solve the governing equations is provided. In applications, the geometry of the shafts and adjoining structures is sufficiently simplified that solutions can be obtained in modest computer run times. Examples using preliminary data from the basalts at the Hanford Site are presented.

INTRODUCTION

The current design of repository facilities for the basalt site includes access shafts ranging in diameter from 1.8 to 3.7 m. At the repository depth (~970 m), these shafts would be connected by access drifts to the rooms where the waste is to be emplaced.

Regulations for repository licensing (10 CFR 60 (1)) require that engineering measures be taken such that, after permanent closure, these shafts are not preferential pathways for radionuclide migration from the repository to the accessible environment. The planned engineering measures currently consist mainly of sealing the drifts and shafts such that potential radionuclide transport through these pathways is reduced to some acceptable design level.

The application of a two-dimensional numerical model for assessing the effectiveness of the drift and shaft seals as impediments to radionuclide migration is described. First a short description of the numerical model is given. Next, application is described. Finally, the results and conclusions are given. The study is somewhat generic in nature, but is useful in identifying the parameters that are important to sealing concepts.

MODEL DESCRIPTION

The numerical model employed in this study is based on three coupled second-order partial differential equations. These equations, describing fluid flow, heat transfer, and mass transport through heterogeneous, anisotropic porous media, are:

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left[K_x \frac{\partial h}{\partial x}\right] + \frac{\partial}{\partial y}\left[K_y\left(\frac{\partial h}{\partial y} + R\right)\right] + m_V + \gamma \frac{\partial T}{\partial t} \qquad (1)$$

$$S_H \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[\left(K_{Tx} + K_{TDx}\right)\frac{\partial T}{\partial x}\right] + \frac{\partial}{\partial y}\left[\left(K_{Ty} + K_{TDy}\right)\frac{\partial T}{\partial y}\right] - S_F \frac{\partial}{\partial x}\left(V_x T\right) - S_F \frac{\partial}{\partial y}\left(V_y T\right) + E_I \qquad (2)$$

$$nR_D \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[n\left(D_x + D_{Mx}\right)\frac{\partial C}{\partial x}\right] + \frac{\partial}{\partial y}\left[n\left(D_y + D_{My}\right)\frac{\partial C}{\partial y}\right] - \frac{\partial}{\partial x}\left(V_x C\right) - \frac{\partial}{\partial y}\left(V_y C\right) + M_C - \lambda n R_D C \qquad (3)$$

where

C = radionuclide concentration (kg/m^3)
D_{Mx}, D_{My} = directional molecular diffusion coefficients (m^2/yr)
D_x, D_y = directional dispersion coefficients (m^2/yr)
E_I = thermal source term (J/m^3-yr)
h = hydraulic head (m)
K_{TDx}, K_{TDy} = directional thermal molecular diffusion coefficients
K_{Tx}, K_{Ty} = directional thermal conductivities (J/yr-m^2-°C/m)
K_x, K_y = directional hydraulic conductivities (m/yr)
M_C = radionuclide source term (kg/m^3-yr)
m_V = volumetric source term (m^3/m^3-yr)
n = porosity of porous medium (m^3/m^3)
R = hydraulic gradient due to thermal buoyancy (m/m)
R_D = retardation coefficient (dimensionless)
S_F = specific heat of fluid (J/kg-°C)
S_H = specific heat of saturated porous medium (J/kg-°C)
S_s = specific storage (1/m)
T = fluid-porous medium temperature (°C)
t = time (yr)
V_x, V_y = directional fluid velocity components (m/yr)
x, y = space coordinates (m)
γ = fluid thermal expansion coefficient (1/°C)
λ = radionuclide decay coefficient (1/yr).

The coupling between the fluid flow (Eq. (1)) and heat transfer (Eq. (2)) in low-permeability media is generally one-way (i.e., the fluid flow is affected by temperature variation (mainly through the buoyancy term, R, in Eq. (1)), but heat transfer is negligibly affected by fluid flow). Derivation of these governing equations is provided in a report by Runchal et al. (2).

To solve the set of governing equations, a regular mesh of rectangular elements is imposed on the domain of interest. A staggered grid pattern is used, in which the dependent variables (h, T, C) are solved for at grid points, while the fluxes of fluid, heat, and radionuclides are computed at midsurfaces (Fig. 1). The method of nodal point integration coupled to the Alternate-Direction-Implicit method is used to obtain the numerical solution. Details of the solution method are provided by Runchal et al. (2). The PORFLO code was used in the sensitivity analysis discussed below. A users manual (3) is available for PORFLO, the computer code which implements the solution. The PORFLO code has been verified and benchmarked (4).

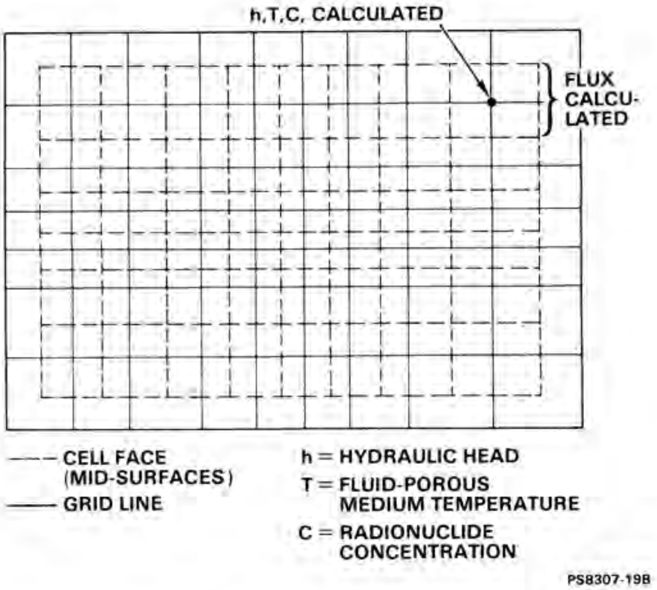


Fig. 1. Example of PORFLO Grid in the Two-Dimensional Cartesian Coordinates.

MODEL APPLICATION

Background

Postclosure repository seals consist of materials and components installed to obstruct potential radionuclide transport pathways through excavated repository openings to the accessible environment. Such potential pathways include shafts, exploratory boreholes, and access and ventilation drifts (Fig. 2). Potential pathways in the damaged rock zone (DRZ) around these excavations, in which hydraulic properties are changed due to the excavation technique, may also require sealing.

The objective of this study was to analyze performance of repository seals as a function of variations in design concepts, site-specific conditions, and material properties. Study results will be used to guide seals component design, test planning, and future modeling approaches. Because of current data and design uncertainties, the intent was to maintain conservatism in all aspects of the analysis.

Performance requirements specified in 10 CFR 60 for repository seals are not quantitative. Hence, for the purposes of this study, a numerical performance measure was specified in terms of a radionuclide flux ratio. This ratio is determined by integrating, over time, the mass flux of a nonsorbing radionuclide entering the shaft at the shaft-access drift intersection, and dividing by a similar, time-integrated (or cumulative) flux of the radionuclide out of the waste emplacement rooms. The basic idea behind this performance measure is to quantify the fraction of radionuclide mass that travels through the seals. A tentative performance goal was set for the fraction to be less than 1% of the U.S. Environmental Protection Agency standard for the total repository system (5). This performance goal is likely to change in the future as the design evolves.

Methods

The numerical study was performed by repeatedly simulating the seals performance for various values of several important parameters. Details of the sensitivity study are available in a report by Seitz et al. (6). The parameters that were varied included:

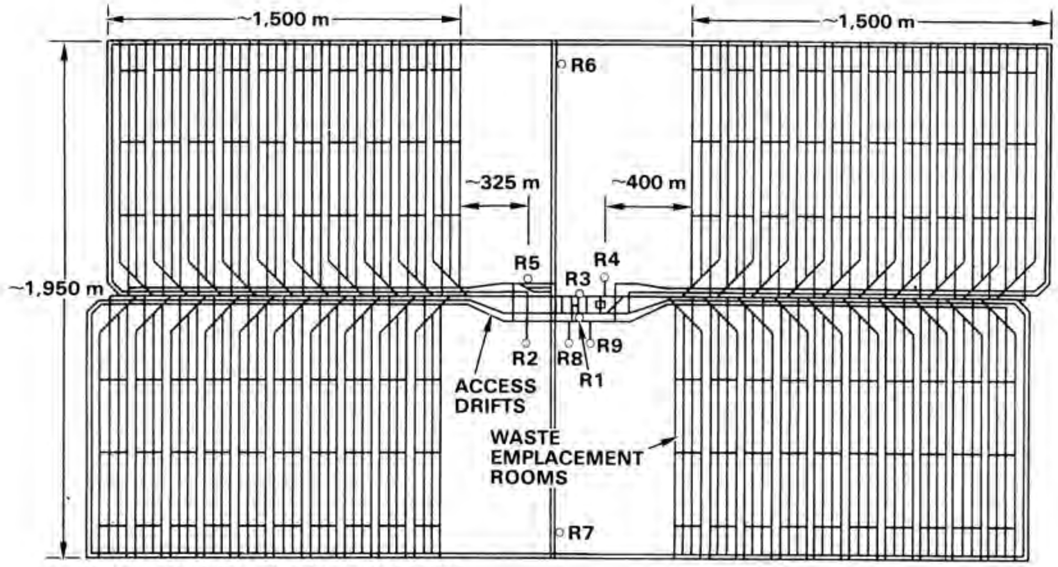
- Length, hydraulic conductivity, and effective porosity of the backfill materials to be placed in the access drifts and waste emplacement rooms
- Hydraulic conductivity of the zone of rock damaged by the excavation of the underground openings
- Presence or absence of radiogenic heat
- Waste package lifetime.

The examples of results that follow are for simulations that indicated significant effects on seals performance.

The two-dimensional conceptual model used for this study is given in Fig. 3. The geometry of the drifts and shafts is three-dimensional; therefore, some liberty was taken in simplifying the problem to fit a two-dimensional model. A version of the two-dimensional model that can accommodate geometrically dissimilar elements and a fully three-dimensional model are currently under development. The primary limitation on using a fine three-dimensional geometry is imposed by requirements of computer memory and time. The repository design assumed for this analysis is currently being revised to include criteria established by Archer (7). Future analyses are planned to assess the effects of these changes on seals performance.

The location and orientation of the vertical cross section depicted in Fig. 3 was selected to provide a relatively high conductivity pathway from the modeled waste emplacement rooms through the access drifts to the shafts. The horizontal hydraulic head gradient is assumed to be oriented parallel to the cross section being modeled, thus forcing the groundwater flow toward the shaft. The distances between the modeled shaft and waste emplacement rooms are defined by the distance from the closest shaft to the emplaced waste in each half of the repository (see Fig. 2). The area between these shafts is ignored.

Dirichlet (fixed) boundary conditions were used at all four boundaries of the conceptual model. The initial hydraulic head values at the boundaries and throughout the domain were based on hydraulic gradients of -0.001 (upward) and -0.0002 (left to right) (8). The initial temperatures were specified based on a temperature of 57 °C at repository depth and a vertical geothermal gradient of -0.04 °C/m (9). For the duration simulated, temperatures at the model boundaries were held at the initial temperatures. The size of the model domain was made sufficiently large that boundary effects on the result were minimized.



NOTE: SHAFTS ARE DENOTED BY CIRCLES.
SHAFTS R4 AND R5 WERE USED TO ESTABLISH DIMENSIONS OF THE COMPUTER MODEL.

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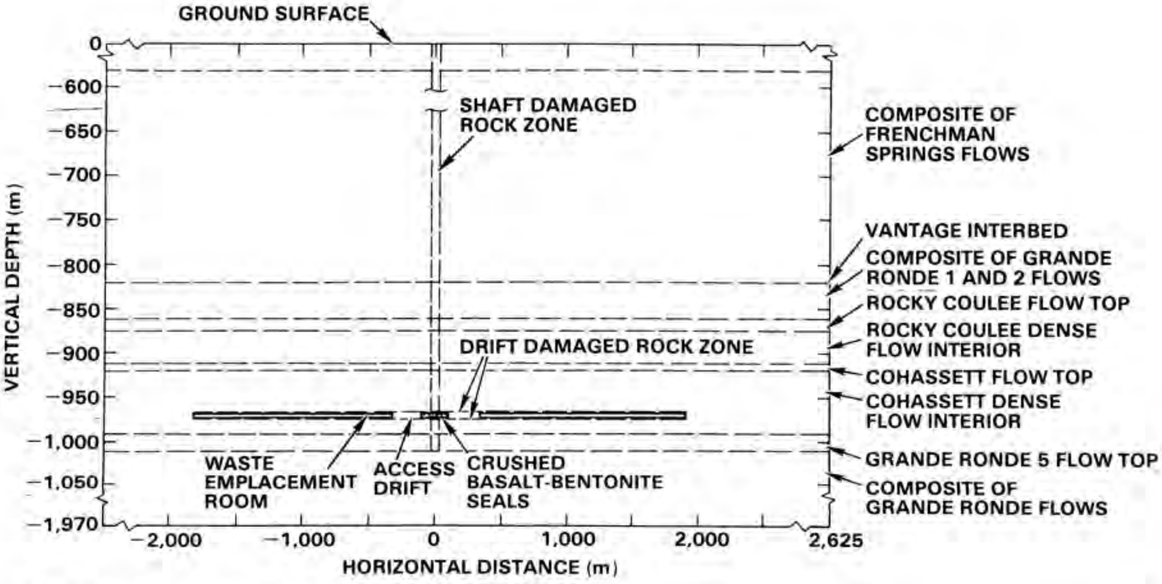
Fig. 2. Plan View of Underground Repository Layout.



NOTE: SHAFT DAMAGED ROCK ZONE IS NOT TO SCALE.

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Fig. 3. Conceptual Model Geometry Used for PORFLO Simulations.

A nonsorbing radionuclide distributed evenly throughout the waste emplacement rooms, and with an infinite half-life, was specified at the time of radionuclide release. The radionuclide concentration is held constant at 6.6 x 10^{-3} kg/m^3 (based on the inventory of Iodine-129 instantaneously distributed throughout the pore space of the waste emplacement rooms). Other input data are shown in Table I. The parameter values assumed for the reference case are listed in Table II.

TABLE I

Selected Data Values Used in Repository Seals Sensitivity Analysis.

Parameter	Value
Hydraulic conductivity of Grande Ronde Basalt dense flow interiors (8, 10)	
Vertical	1.5 x 10^{-12} m/s
Horizontal	5.0 x 10^{-13} m/s
Hydraulic conductivity of Cohassett flow top* (9, 11)	2.0 x 10^{-8} m/s
Hydraulic conductivity of other Grande Ronde Basalt flow tops* (9, 11)	2.0 x 10^{-7} m/s
Hydraulic conductivity of crushed basalt (12)	10^{-4} to 10^{-5} m/s
Hydraulic conductivity of 75% crushed basalt-25% bentonite (13)	10^{-7} to 10^{-9} m/s
Effective porosity of Grande Ronde Basalt dense flow interiors (9, 14)	0.0001
Effective porosity of Grande Ronde Basalt flow tops (9, 14)	0.005
Effective porosity of 75% crushed basalt-25% bentonite (13)	0.38

*Assumed to be isotropic.

TABLE II

Reference Case Parameter Values.

Parameter	Value
Length of seal	30.5 m
Waste package life	1,000 yr
Hydraulic gradient	Natural + induced*
Hydraulic conductivity (K) of damaged rock zone (15)	1,000 x host rock K
Crushed basalt	
Hydraulic conductivity	10^{-4} m/s
Effective porosity (12)	0.50
75% crushed basalt-25% bentonite	
Hydraulic conductivity	10^{-9} m/s
Effective porosity	0.38

*Radiogenic heat is considered.

The finite-difference grid used for this analysis consisted of 19 material types, defined by 79 nodes on the x-axis and 50 nodes on the y-axis, yielding a total of 3,950 nodes to characterize the domain. The 10,000-yr simulations were divided into two parts: (1) the time before waste package failure, during which the coupled groundwater flow and heat transfer equations were solved, and (2) the time after waste package failure, during which the coupled groundwater flow, heat transfer, and radionuclide transport equations were solved. The numerous time steps required for a 10,000-yr simulation, in conjunction with the large number of nodes, resulted in run times of approximately 20 to 30 central processing unit hours on the Basalt Waste Isolation Project Prime 750 computers. The same runs required approximately 15 central processing unit minutes on a Cray-1 computer.

Results

Temperatures and Buoyancy Gradients.

The PORFLO simulations produce plot files that allow the user to extract temperatures or groundwater density for any point in the model domain at the times specified. By using postprocessors, the plot files can be displayed as cross-sectional isothermal curves or isothermal surfaces. Examples are given in Fig. 4 and 5. As shown in the figures, most of the heat generated by the emplaced waste is confined to the regions directly above and below the modeled waste emplacement rooms. Therefore, the increase in temperature at the shaft is less than the increase near the waste emplacement rooms. The temperatures as a function of space and time are shown in Fig. 6. From this figure, it is apparent that the temperature at the shaft is less than the temperature near the waste emplacement rooms for the duration of the simulation. However, the difference between the temperatures at these two locations decreases after 1,000 yr.

The hydraulic gradient due to thermal buoyancy at repository depth for the shaft and the waste emplacement rooms is shown in Fig. 7. The magnitude of the buoyancy is significant compared to the magnitude of the natural hydraulic gradient (0.001). The sum of these two terms is the total vertical driving force (per unit weight). Because temperatures are greater near the waste emplacement rooms, the buoyancy forces are greater there than at the shaft. The magnitude of this force at both locations indicates that it would not be conservative to analyze performance of the seals while neglecting the thermal component of the vertical driving force.

Contaminant Plumes.

The PORFLO code also generates contour plot files for concentrations of a specified contaminant at given times. Postprocessors can be used to generate isoconcentration contours from these files. Contours for the reference case at 100 yr after waste package failure are shown in Fig. 8 and 9. The contaminant plumes migrate toward the shaft, suggesting that the flow interior resists groundwater transport sufficiently well to force the radionuclides toward the more permeable shaft. The spreading of the contaminant plume upward and downward into the dense flow interior indicates that molecular diffusion may account for a significant amount of the flux that appears in the denominator of the radionuclide flux ratio.

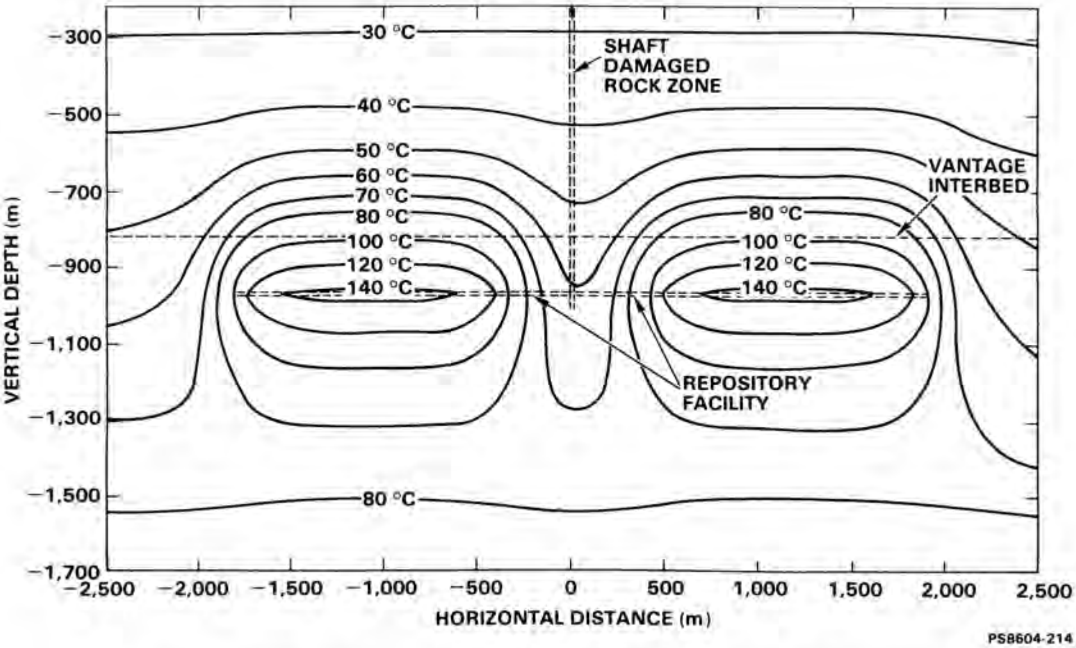


Fig. 4. Isotherms at 1,000 yr after Waste Emplacement (vertical section).

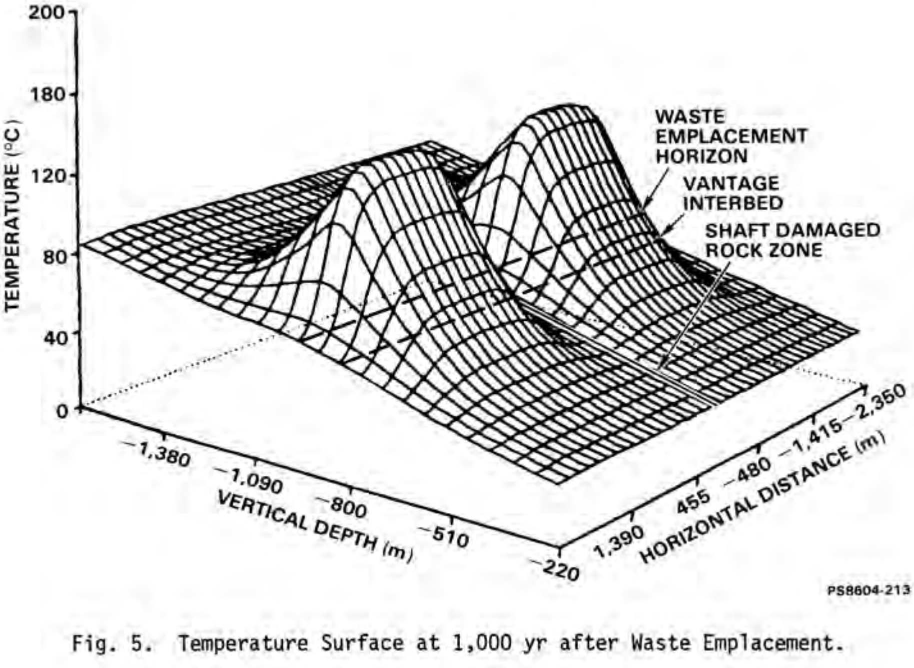


Fig. 5. Temperature Surface at 1,000 yr after Waste Emplacement.

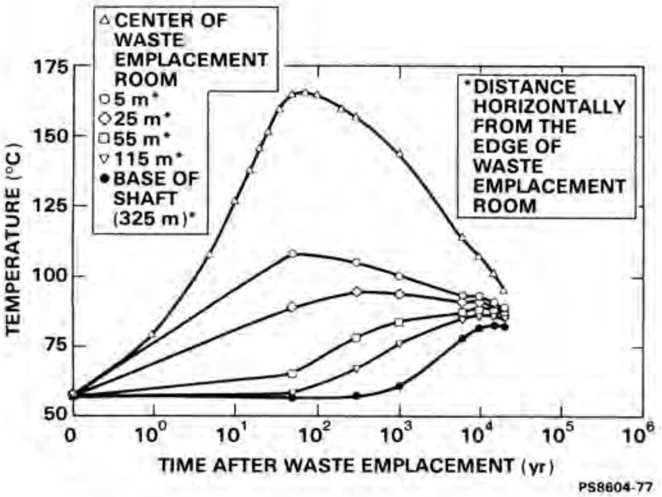


Fig. 6. Temperatures at Repository Depth.

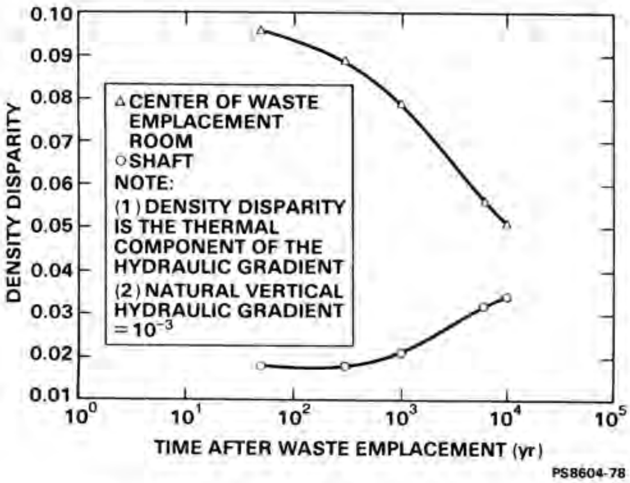
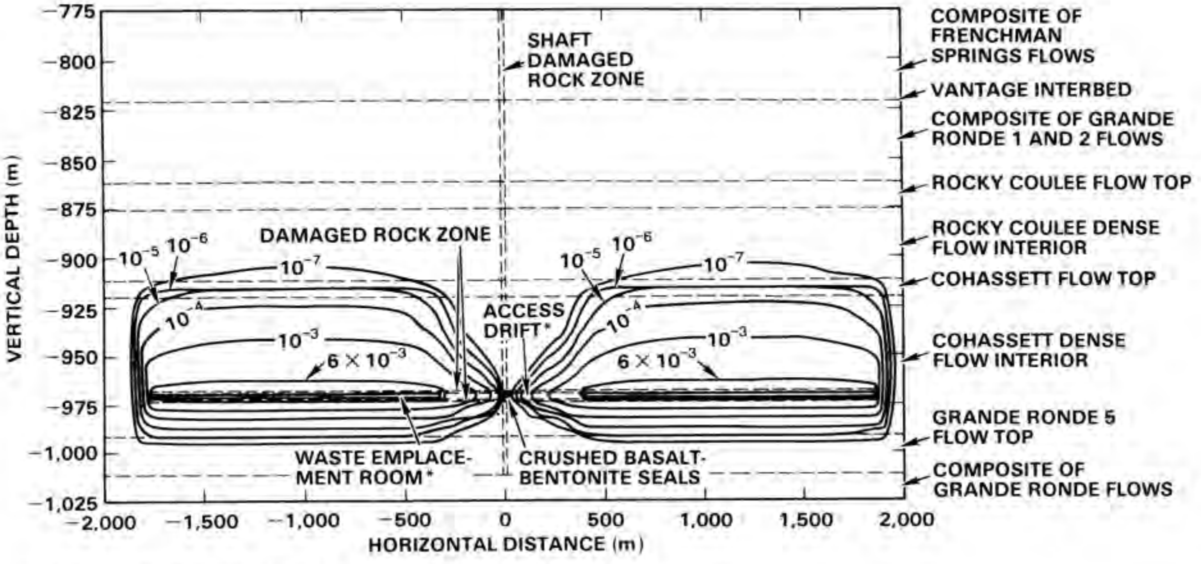


Fig. 7. Density Disparity of Groundwater at Repository Depth.



NOTE: UNITS OF CONCENTRATION CONTOURS = kg/m³.
SHAFT DAMAGED ROCK ZONE IS NOT TO SCALE.
FOR CONDITIONS AT 100 yr AFTER CONTAINER FAILURE (1,100 yr AFTER WASTE EMPLACEMENT).
*CRUSHED BASALT BACKFILL

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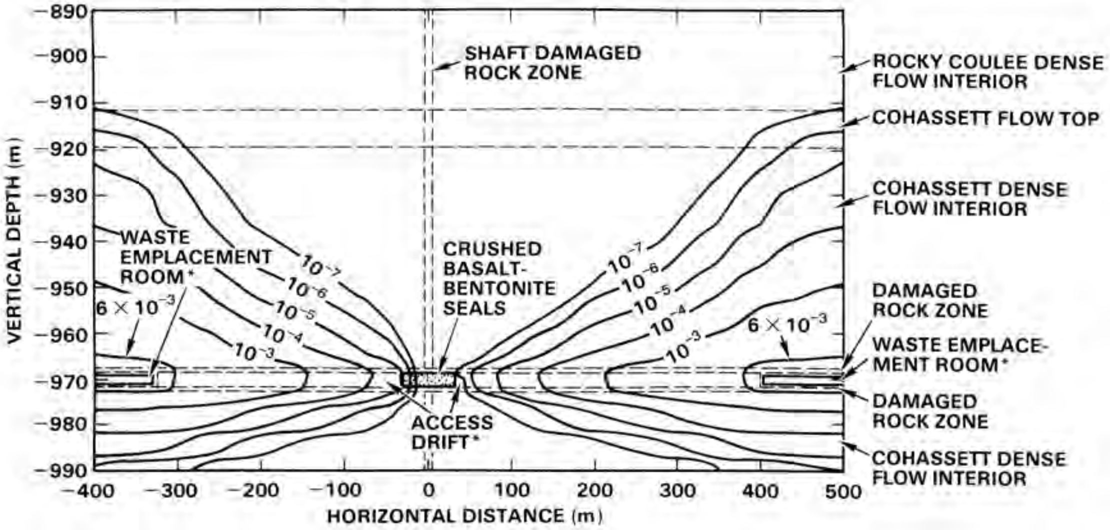
Fig. 8. Contaminant Plume Isoconcentration Contours for Reference Conditions.



NOTE: UNITS OF CONCENTRATION CONTOURS = kg/m^3.
SHAFT DAMAGED ROCK ZONE IS NOT TO SCALE.
FOR CONDITIONS AT 100 yr AFTER CONTAINER FAILURE
(1,100 yr AFTER WASTE EMPLACEMENT).
*CRUSHED BASALT BACKFILL

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Fig. 9. Detail of Contaminant Plume Isoconcentration Contours for Reference Conditions.

Radionuclide Flux Ratios.

The radionuclide flux ratio was recorded as a function of time for each simulation. These ratios were then plotted to depict the effects of changes in input parameter values. Changes in the flux ratio as a function of seal hydraulic conductivity and effective porosity, and as a function of DRZ hydraulic conductivity, are shown in Fig. 10 and 11, respectively. Changes in the hydraulic conductivity of the seal material and the DRZ caused the most change in the radionuclide flux ratio.

The results shown in Fig. 10 suggest that a seal hydraulic conductivity as high as 10^{-7} m/s may be sufficient to maintain performance within allowable limits. Laboratory tests have demonstrated that seal hydraulic conductivities as low as 10^{-11} to 10^{-12} m/s may be attainable (13). The results shown in Fig. 11 suggest that a DRZ hydraulic conductivity more than 1,000 times greater than the hydraulic conductivity of the undisturbed dense flow interior may not be acceptable. Past studies have shown that the maximum hydraulic conductivity for the DRZ should not exceed 1,000 times that of the surrounding host rock (15). None of the other cases in which a seal was present in the drifts produced results that exceeded the allowable radionuclide flux ratio. A complete description of these results is available in Seitz et al. (6).

SUMMARY AND CONCLUSIONS

Sensitivity of repository seals performance was studied through the application of a two-dimensional numerical analysis computer code (PORFLO). Several simplifying assumptions were made to accommodate the three-dimensional geometry of the repository in a two-dimensional model. In addition, there is considerable uncertainty in currently available data and designs. The study nevertheless provides a useful ranking of parameters that are important to the performance of the seals.

The results of the sensitivity analysis demonstrate that the hydraulic conductivity of the seal material and the DRZ are the parameters to which seals performance is most sensitive. Predicted releases approached or violated the performance goal when bounding values were used for these parameters. However, performance of the repository seals is well within the acceptable range for expected material properties.

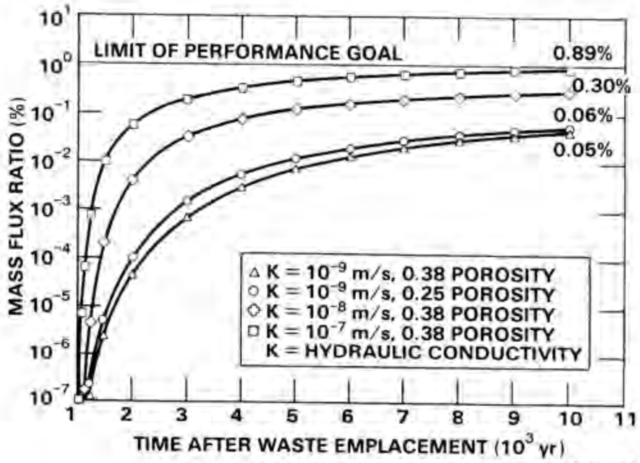

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Fig. 10. Radionuclide Flux Ratios as a Function of Hydraulic Conductivities of Crushed Basalt-Bentonite Backfill for Crushed Basalt Hydraulic Conductivity of 10^{-4} m/s

More realistic studies of seals performance using improved models are planned. These include a two-dimensional model in which the drifts and shafts will be represented as circular one-dimensional directed elements in a two-dimensional field. In this approach, the flow and transport through these elements would be solved independent of the two-dimensional porous medium elements. Alternatively, a fully three-dimensional model with similar shaft elements is under development. The primary aim of all these developments is to perform realistic simulations within available computer resources.

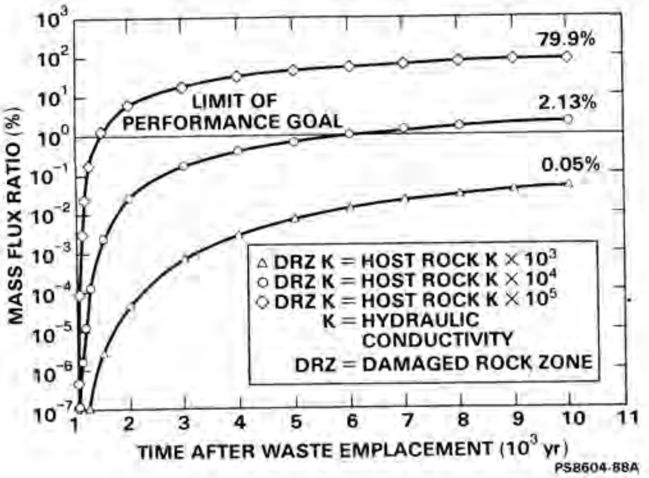

Fig. 11. Radionuclide Flux Ratios as a Function of Damaged Rock Zone Hydraulic Conductivity.

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