

FINITE-ELEMENT THERMOHYDROGEOLOGICAL MODELING FOR CANADIAN NUCLEAR FUEL
WASTE MANAGEMENT

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ABSTRACT

A three-dimensional finite-element code, MOTIF, has been developed to simulate the coupled processes of groundwater flow, heat transfer and solute transport. This MOTIF code is applied to simulate the migration of inert contaminants from a hypothetical nuclear fuel waste vault through the geosphere to the biosphere. The conceptual model used in this simulation is consistent with surface and subsurface geological, geophysical and hydrogeological data from the granite batholith and surrounding country rock that comprise the Whiteshell Research Area in eastern Manitoba, Canada.

INTRODUCTION

The Canadian Nuclear Fuel Waste Management Program is currently assessing the concept of disposing of nuclear fuel waste deep within plutonic rock. A Monte Carlo simulation code, SYVAC (System Variability Assessment Code) is being applied to assess the radiological impact of geological disposal. (1) Due to the large number of sampled runs required for Monte Carlo simulation, the geological system has to be represented by a highly idealized model. This precludes a direct comparison of SYVAC predictions with field data. It is, however, still possible to make an indirect connection by first constructing a detailed model based on laboratory and field data to simulate the transport of contaminants from the nuclear fuel waste vault through the geosphere to the biosphere. The results of the detailed model are then utilized to construct a simplified SYVAC model. It is the purpose of this paper to describe the development of the detailed geosphere model and present some preliminary simulation results.

The strategy for developing the simplified geosphere transport model for SYVAC is discussed in Section 2. Section 3 outlines the mathematical and numerical aspects of the finite-element code MOTIF (Model of Transport in Fractured/Porous Media) as well as its verification and validation. This is followed by a discussion of a detailed conceptual hydrogeological model of the geosphere based on field data from the Whiteshell Research Area in Section 4, heat and groundwater flow simulation in Section 5, and preliminary transport simulation in Section 6. Finally, some conclusions are drawn in Section 7.

GEOSPHERE MODELING STRATEGY

The overall disposal system assessment model in SYVAC consists of three submodels:

- (1) a vault submodel to simulate the release of contaminants from the waste package and their transport through the buffer material,

- (2) a geosphere submodel to simulate the movement of contaminants through the subsurface rocks and saturated soils,
- (3) a biosphere submodel to simulate the movement of contaminants through the near-surface and surface environment and to calculate the consequent toxic or radiological dosage to biological species.

The present paper is concerned with the geosphere.

As illustrated in Figure 1, the development of the SYVAC geosphere submodel comprises the following steps:

- (1) construction of a conceptual model of the subsurface structure and hydrogeology consistent with geological, geophysical and hydrogeological data from field investigations in a research area, as well as material properties determined in laboratory testing,

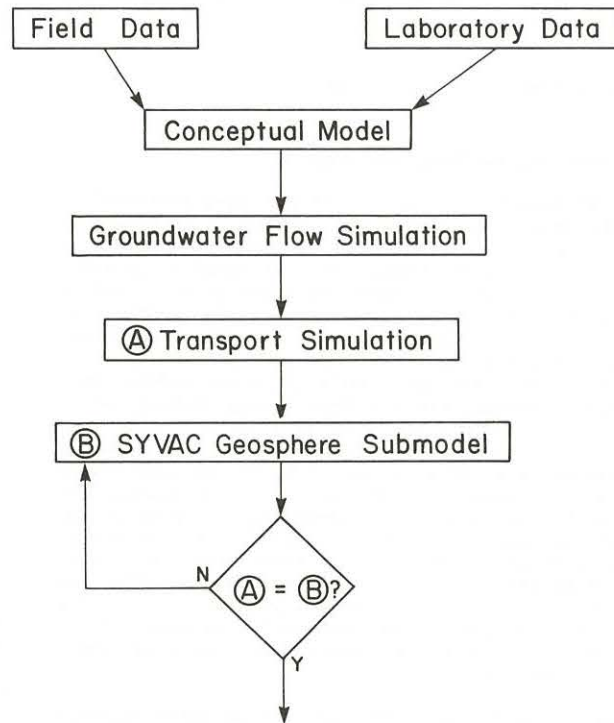


FIGURE 1: STRATEGY FOR DEVELOPING THE GEOSPHERE SUBMODEL IN SYVAC

- (2) detailed simulation of groundwater flow through the geosphere under the driving forces of gravity and thermal buoyancy,
- (3) detailed simulation of convective, diffusive and dispersive transport of contaminants through the geosphere, and
- (4) development of a simplified SYVAC geosphere submodel compatible with the results of the detailed model in steps 2 and 3 above.

This approach to developing a disposal system assessment model has been discussed in some detail by Dormuth and Lyon. (2) The detailed geosphere modeling, which is performed by applying the MOTIF finite-element code (see Section 3 below), predicts the spatial distribution and temporal evolution of temperature, piezometric head and contaminant concentration. Some of these results can be compared with data from field experiments or observations. The initial SYVAC geosphere submodel being developed is a one-dimensional network. Some of its input parameters such as transport path geometry and groundwater velocities have to be determined from the results of the MOTIF geosphere model. Other input parameters such as diffusion and dispersion coefficients are chosen to conform to those input to the MOTIF geosphere model. The SYVAC submodel predicts the contaminant discharge rate (integrated mass flux) at various points in the network of paths. This can be compared with the results of the MOTIF geosphere model. The final SYVAC submodel is to be determined in an iterative manner, as illustrated in Figure 1, until its predictions agree sufficiently well with the MOTIF model. Subsequently, certain processes such as radioactive decay chain, physical or chemical retardation, or other rock-water-waste interactions, which may not be simulated efficiently in the detailed geosphere model, can also be included in the SYVAC submodel.

THE MOTIF FINITE-ELEMENT CODE

Mathematical and Numerical Aspects

A finite-element code MOTIF has been developed at Atomic Energy of Canada Limited (AECL) to solve the steady-state and transient problems of groundwater flow, contaminant (including one-species radionuclide) transport, and heat transport in saturated or partially saturated fractured or porous media. (3) The MOTIF code solves the three partial differential equations governing these physical phenomena, i.e., the fluid mass balance equation, the contaminant mass balance equation and the heat energy balance equation. The fluid flow is assumed to be laminar and sufficiently slow that momentum conservation can be approximated by Darcy's law. (4) In the generalized fluid mass balance equation, the fluid density and viscosity can vary with temperature, pressure and solute or contaminant concentration. In the energy balance equation, conductive, dispersive and convective heat transfer mechanisms are included. Similarly, the solute mass balance equation accounts for diffusive, dispersive and convective transport mechanisms. Therefore, the flow and transport processes are generally coupled.

In the MOTIF code, the Galerkin weighted residual method, in conjunction with the finite-element approximation, is utilized for spatial discretization. This renders each governing equation into a system of

ordinary differential equations. Finite-difference approximation for the temporal derivatives further reduces each into a sparse set of simultaneous linear algebraic equations. The time-integration scheme incorporated in MOTIF enables the user to specify fully explicit, Crank-Nicholson or fully implicit finite difference, or any scheme in between. The three sets of equations for flow, solute transport and heat transport are solved sequentially, as illustrated in Figure 2, using a numerical algorithm based on Gaussian elimination. Solution of the flow equation provides the spatial distribution and time evolution of hydraulic head or, equivalently, pressure and velocity. The latter is fed into the convection terms in the solute transport and heat transport equations. The pressure, p , temperature, T , and concentration, C , solutions are substituted into the constitutive equations to update the values of fluid density, ρ , and viscosity, μ , before advancing to the next time step. A Picard iteration loop is incorporated within the time-marching cycle to handle very nonlinear problems.

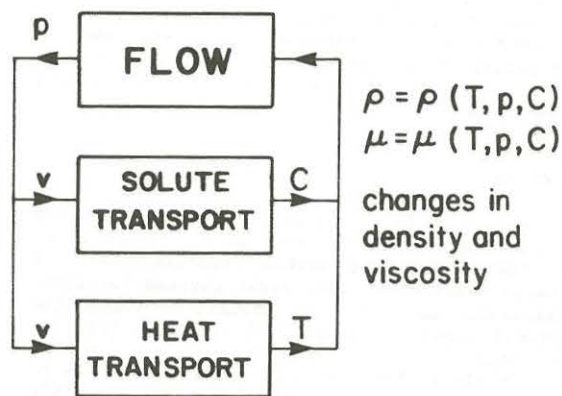


FIGURE 2: SCHEMATIC REPRESENTATION OF THE MOTIF ALGORITHM FOR SOLVING THE COUPLED PROCESSES OF GROUNDWATER FLOW, SOLUTE TRANSPORT AND HEAT TRANSPORT

Linear sorption and radioactive decay for one species can also be simulated using MOTIF. Such complications, however, are omitted in the initial stage of geosphere modeling reported herein. Furthermore, for the present application the contaminant concentration is expected to be very low. The variation of viscosity with hydraulic pressure to a depth of several km is also insignificant. Consequently, the constitutive equations assume the simplified forms $\rho = \rho(T, p)$, $\mu = \mu(T)$.

Available Element Types

As illustrated in Figure 3, three types of isoparametric elements are available in MOTIF: a hexahedron, a 2-D quadrilateral and a 1-D line element. These elements are all defined in a 3-D space, thus the hexahedron element can be used to represent porous media in a 3-D model while the quadrilateral element can be used either to represent porous media in a 2-D model or planar fractures or fracture zones in a 3-D model. Similarly the line element can be used to represent porous media in a 1-D model, or planar fractures or fracture zones in a 2-D model, or narrow

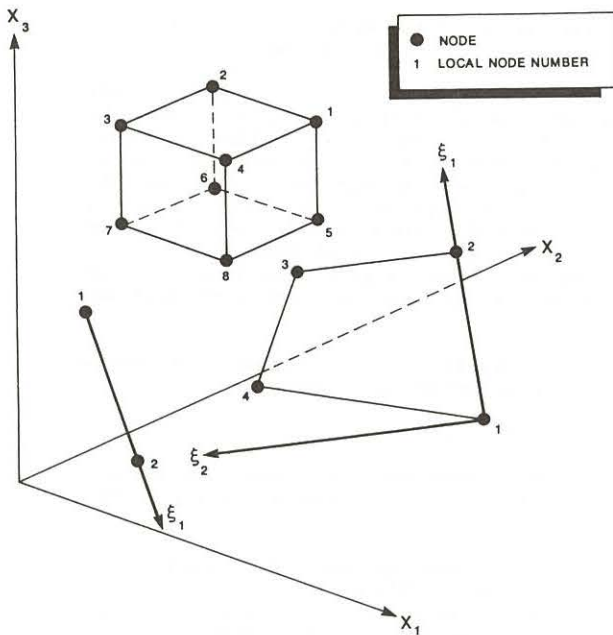


FIGURE 3: TYPES OF FINITE ELEMENTS AVAILABLE IN MOTIF: AN 8-NODED HEXAHEDRON, A 4-NODED QUADRILATERAL AND A 2-NODED LINE

channels and pipes in a 3-D model. A combination of these can be employed in a single model.

Verification

For quality assurance the MOTIF code has been verified by comparison with analytical solutions for the following problems:

- (a) a semi-infinite strip recharge basin,
- (b) a pumping well intersected by a vertical fracture plane,
- (c) a finite, confined circular aquifer with an injection well intersected by a horizontal fracture plane,
- (d) a one-dimensional radionuclide transport with hydrodynamic dispersion, linear absorption, and radioactive decay,
- (e) one-dimensional heat transport, and
- (f) hydrothermal convection around an exponentially decaying spherical heat source.

In addition, the MOTIF solutions have been compared with other numerical solutions for

- (a) thermal buoyancy flow,
- (b) concentration-driven flow and
- (c) topographically driven steady-state flow in a porous medium traversed by two intersecting fracture zones.

Most of the verification cases listed above were discussed in reference 5.

Validation

As a major validation exercise, the MOTIF code was employed to predict in advance the hydraulic perturbations caused by the excavation for a large underground experimental facility for Canada's Underground Research Laboratory (URL) in a granitic pluton in Manitoba. Preliminary comparisons have been made between model predictions and some of the observed piezometric responses. (6,7) In general, the predicted drawdown histories agree well with observations.

CONCEPTUAL HYDROGEOLOGICAL MODEL OF THE WHITESHELL RESEARCH AREA

The Whiteshell Research Area covers about 750 km² in southeastern Manitoba (Figure 4) including the sites of the Whiteshell Nuclear Research Establishment (WNRE) and the URL. A major portion of the area consists of part of the Lac du Bonnet Batholith, a large granitic pluton. In general the topography slopes from elevations of 300 m above sea level in the southeast to 250 m in the northwest.

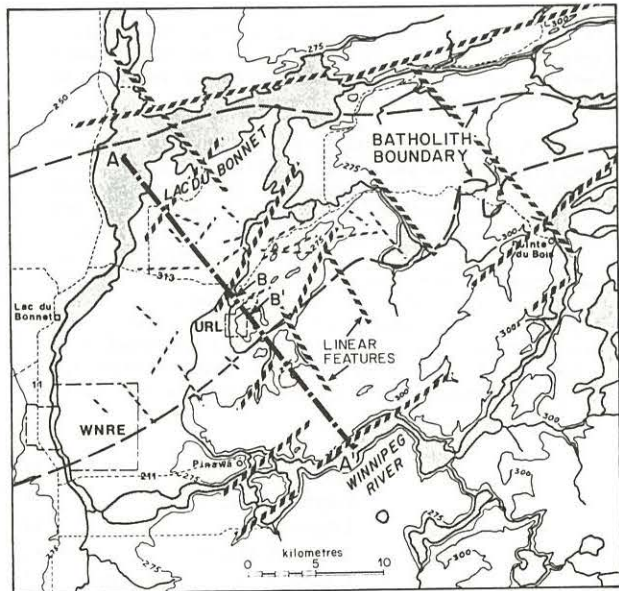


FIGURE 4: TOPOGRAPHIC MAP OF THE WHITESHELL RESEARCH AREA. ALL CONTOURS IN METRES ABOVE SEA LEVEL. SECTIONS BB' AND AA' ARE SHOWN IN FIGURES 5 AND 6, RESPECTIVELY

The Winnipeg River system is assumed to provide a stable hydrogeological boundary nearly surrounding the area. The water table reflects the topography.

Until recently subsurface investigations in boreholes were limited to the WNRE and URL sites. Features and properties controlling groundwater flow were determined from borehole logs and hydrogeological testing and monitoring.

Figure 5 shows a NW-SE oriented cross section of the geology at the URL site. Three low-dipping fracture zones appear to be the predominant controls on groundwater flow. The presence of two vertical fracture zones is inferred from hydrogeological responses and surface traces of linear features.

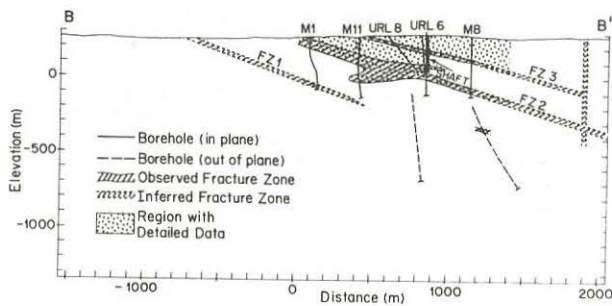


FIGURE 5: SECTION BB' (SEE FIGURE 4) SHOWING OBSERVED AND INFERRED GEOLOGY NEAR THE URL

The area that must be modeled to analyze the impact of a waste disposal vault is much larger than that for which detailed data is currently available. Therefore the conceptual model has been extended based on the information at the WNRE and URL sites and assumptions about linear features detected from aerial photography and geophysics. (8) The linear features in Figure 4 are assumed to be subvertical fracture zones, the major ones being at least 4 km deep and the minor ones 1 km deep.

Figure 6 is an extension of the previous cross section through the URL site showing the conceptualized geology. Low-dipping fracture zones are assumed to intersect the surface at vertical zones. Most are extended to intersect another vertical zone at depth. This is to permit the analysis of a regionally continuous fracture zone system, a conservative assumption with regards to radionuclide transport. The fracture zones are considered to be porous media and uniform in thickness. The rock mass is divided into five layers of porous media with permeability and porosity decreasing with depth. The permeability

Layer 1		$K_H = 10^{-15} \text{ m}^2, K_V = 5 K_H, \theta = 0.005$
Layer 2		$K_H = 10^{-17} \text{ m}^2, K_V = 5 K_H, \theta = 0.004$
Layer 3		$K_H = 10^{-19} \text{ m}^2 = K_V, \theta = 0.003$
Layer 4		$K_H = 10^{-20} \text{ m}^2 = K_V, \theta = 0.003$
Layer 5		$K_H = 10^{-21} \text{ m}^2 = K_V, \theta = 0.003$
Fracture Zone		$K_L = 10^{-13} \rightarrow 10^{-19} \text{ m}^2, \theta = 0.1 \rightarrow 0.005$
Zone		$K_T = 0.2 \rightarrow 1.0 K_L$

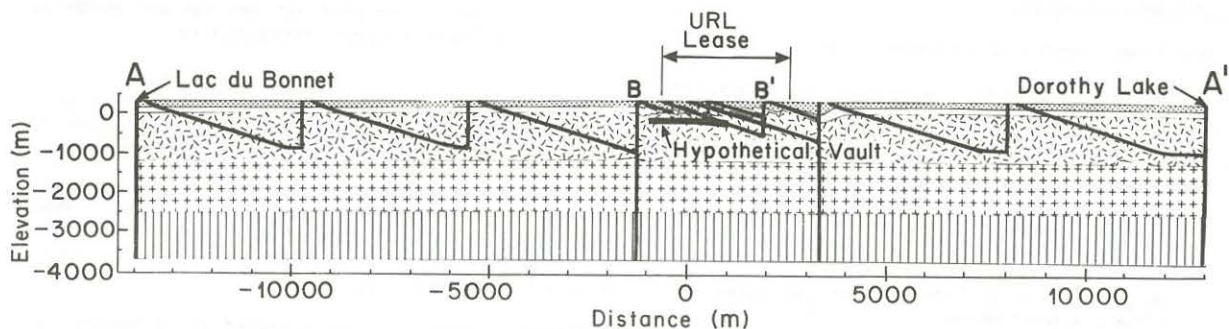


FIGURE 6: CONCEPTUALIZED GEOLOGY ALONG SECTION AA' OF FIGURE 4 FOR 2-D MODELING

of the fracture zones is two to four orders of magnitude higher than that of the rock mass.

It is important to note that the conceptual model is one possible interpretation based on available data. It has been constructed to allow sensitivity analyses with respect to assumptions about features and their properties. As more data becomes available it will be used to improve and hopefully validate the model. Considerable confidence in the modeling approach has already been gained from the success in simulating the hydrogeological impact of the construction of the URL shaft where more geological data existed. (6,7)

Additional details on the conceptual model can be found in Scheier and Whitaker. (9)

FLOW SIMULATION

Coupled fluid flow and heat transport in the conceptual model are being simulated using the MOTIF code.

A hypothetical used fuel vault, 1.9 km x 1.9 km is located at a depth of 500 m (Figure 7). It is purposely located to intersect a fracture zone to assess the effect of fracture proximity. The heat output of the vault is initially 11.6 W/m² and decays to 0 in 100 000 years. The rock is assigned a thermal conductivity of 3.34 W/m·°C and a specific heat of 800 J/kg·°C.

Several 2-D and 3-D finite-element representations of the conceptual model have been constructed. The top boundary of the mesh has prescribed head values equal to water table elevations. The bottom boundary is assumed to be impermeable and the side no-flow due to symmetry. All boundaries have prescribed temperatures based on geothermal measurements at the URL. (10)

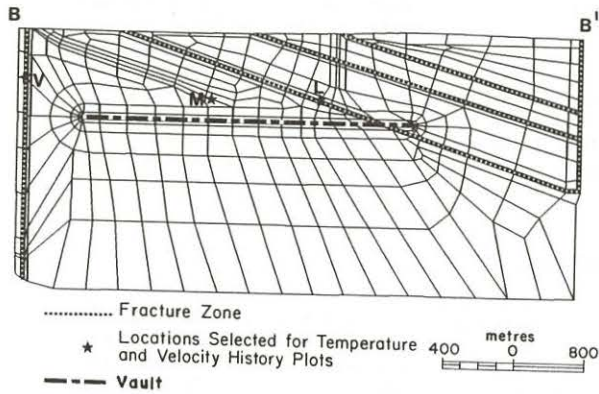


FIGURE 7: TWO-DIMENSIONAL FINITE-ELEMENT MESH - VAULT REGION

Two-Dimensional Modeling

Initially a 2-D model corresponding to the cross-section of Figure 6 was constructed to help define an adequate 3-D representation, select a suitable form for the SYVAC geosphere submodel and assist in sensitivity analysis. This 27 km x 4 km section is essentially along a flow line, i.e., there is little flow perpendicular to the plane. All major fracture zones and stratigraphy of the conceptual model are included. Element properties such as permeability and porosity have been selected initially as average values for the units in the conceptual model but are adjusted for sensitivity analysis.

To check numerical convergence of predictions, two meshes and three time-stepping sequences of differing refinement were used in this analysis. All elements were 2-D. Figure 7 illustrates the coarse-mesh option for the vault region. Small elements are used near the vault and fracture zones with a progressive increase in size further away. This is to ensure accurate calculation of groundwater velocities along likely radionuclide pathways. The coarse mesh consists of a total of 914 quadrilateral elements and 985 nodes. The fine mesh has been constructed by dividing each element of the coarse mesh in four.

Transient simulations are conducted for a period of one million years using geometrically increasing time steps. The coarse time stepping sequence consisted of 20 steps, the medium 42 and the fine 81.

The numerical convergence study showed that the coarse mesh and medium time-stepping sequence are suitable for modeling purposes. Further refinement resulted in only small changes in reference head and velocity predictions and virtually identical temperature predictions.

Example predictions of temperature and velocity components near the vault are shown in Figure 8. Locations M and L are about 100 m above the vault in the rock mass and in the low-dipping fracture zone that intersects the vault, respectively (see Figure 4). Location V is about 200 m above the vault in a vertical fracture zone 325 m from the edge of the vault.

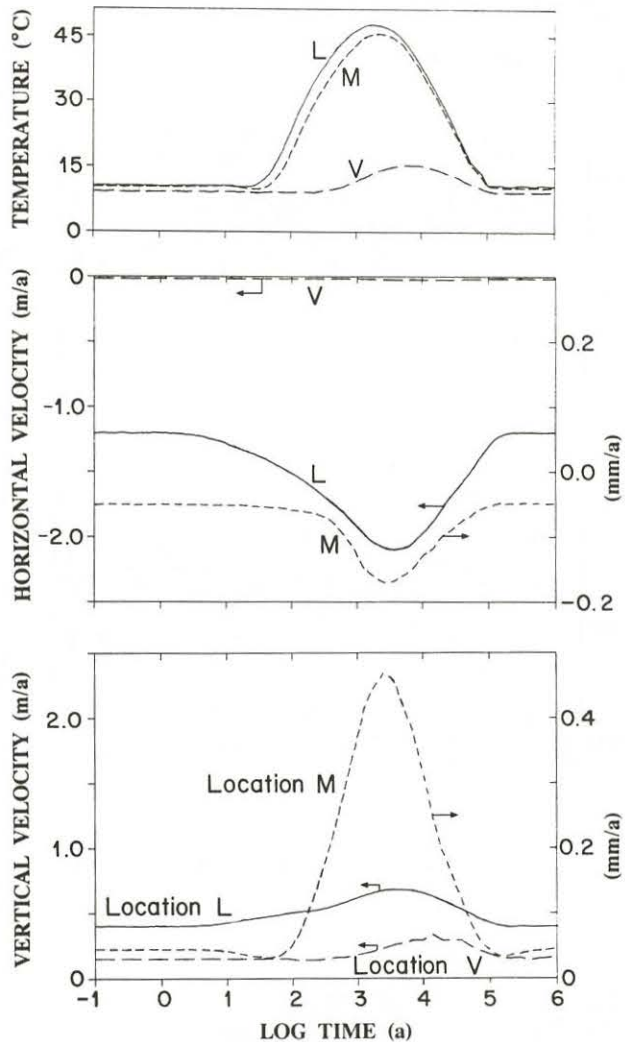


FIGURE 8: PREDICTED TEMPERATURE AND VELOCITY NEAR THE VAULT

For this simulation the velocity in fracture zones near the vault is of the order of 1 m/a. In the rock mass outside the fracture zones, velocities are typically four orders of magnitude lower.

In general the perturbation in both temperature and velocity lasts about 100 000 years. The temperature rise extends about 2000 m from the vault, with convective heat transport being negligible. The peak temperature is 70°C at the vault centroid after 60 years and rapidly decreases and is delayed at points further away. The velocity peak slightly lags that in temperature. In the rock mass at the vault centroid the peak velocity is approximately 20 times the initial value. This increase drops off rapidly with distance. In fracture zones near the vault the velocities increase to about twice the steady-state values.

Figure 9 shows the predicted velocity vector pattern near the vault. The steady-state pattern is

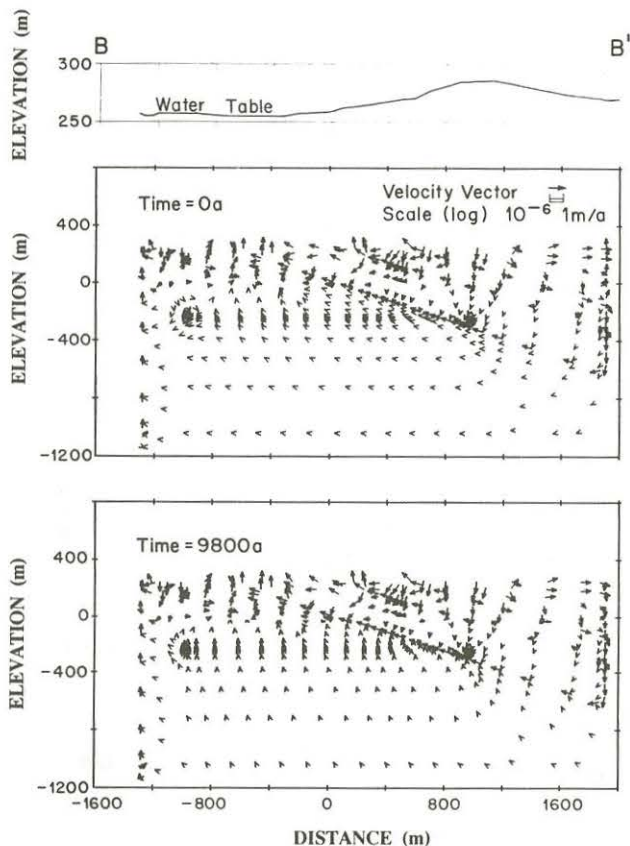


FIGURE 9: WATER TABLE PROFILE AND PREDICTED VELOCITY DISTRIBUTION NEAR THE VAULT

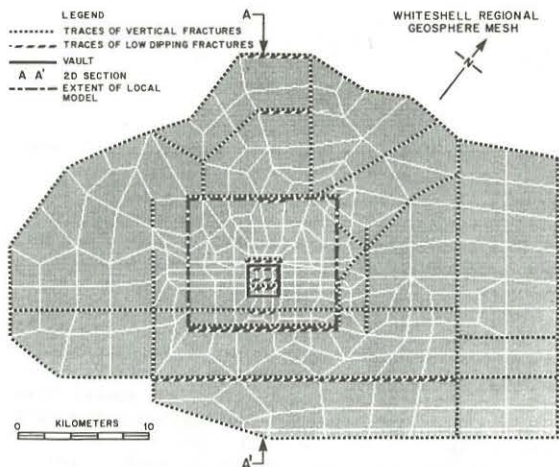


FIGURE 10: PLAN VIEW OF THE FINITE-ELEMENT MESH FOR THE 3-D REGIONAL GEOSPHERE MODEL. FRACTURE TRACES ARE INDICATED BY DOTTED LINES FOR VERTICAL FRACTURES AND BY DASHED LINES FOR THE LOW DIPPING FRACTURE. THE SOLID SQUARE LINE INDICATES THE POSITION OF THE VAULT WHILE AA' CORRESPONDS TO AA' OF FIGURE 4. THE DOT-DASHED LINE INDICATES THE EXTENT OF THE LOCAL MODEL.

nearly semi-circular with recharge in the higher area in the southeast, lateral movement above the lower permeability layers at depth and discharge up through the left side of the vault to the low-lying area in the northwest. The local surface topography (as reflected in the water table) drives the flow. Flow is up the low-dipping fracture zone intersecting the vault. At 9800 a the overall perturbation in velocity field is near its maximum. The flow pattern is now nearly vertical through almost the entire vault due to the buoyancy effect of the waste heat.

Three-Dimensional Modeling

Due to the very large area covered by the Whiteshell Research Area, a 3-D finite-element mesh that can cover the whole area would be rather coarse. A finite-element analysis based on such a mesh could not be expected to produce reliable predictions for the area near the vault.

A two-stage approach is, therefore, adopted whereby a regional model with a coarse mesh is employed to simulate the entire research area and a local model with a refined mesh is used for detailed simulation near the vault. Results from the regional model are used to define boundary conditions for the local model.

The regional geosphere model for the Whiteshell Research Area covers the area bounded by the Winnipeg River system shown in Figure 4 and extends to a depth of 4 km.

A plan view of the finite-element mesh is shown in Figure 10. All lines indicate element boundaries in a single horizontal slice. The background rock is represented by 3432 3-D elements forming eleven geometrically identical horizontal layers. Fracture traces are indicated by dotted lines for vertical fractures and by dashed lines for the low dipping fractures. The fractures are represented by planar 2-D elements. There are 1919 planar elements, sharing nodal points with some of the 3D elements. The solid square line indicates the position of the vault while AA' in Figure 10 corresponds to AA' in Figure 4. The dot-dashed line indicates the plan view extent (8.5 km x 10 km) of the local model.

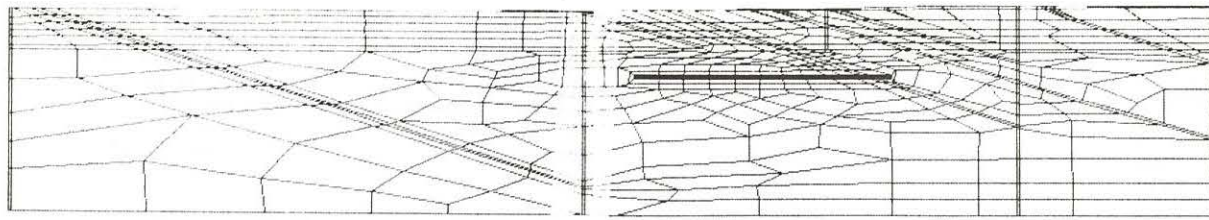
The local model extends to a depth of 1.5 km. The finite-element mesh consists of 6864 nodes and 5840 3-D elements. It is constructed by repeating 12 times the layer of nodal points in the NW-SE section shown in Figure 11. Fracture zones can be recognized by double lines while the elements representing the vault are indicated by the dark area in the central portion of the mesh.

A preliminary case of the local 3-D geosphere model has been run and analysed. Particle track results indicate somewhat longer transit times than those obtained from the 2-D modeling.

Sensitivity Analysis

Analysis of the sensitivity of predicted flows near the vault is being done using both 2-D and 3-D models. Factors being examined include numerical discretization, variation in the location and nature of boundary conditions, variations in the fracture zone conceptualization, values of parameters such as hydraulic conductivity and porosity assigned to

WHITESHELL GEOSPHERE LOCAL 3D MODEL



NW to SE Section Through The Vault

0 METRES 1000

FIGURE 11: NW TO SE SECTION THROUGH THE VAULT SHOWING VERTICAL SECTION FINITE-ELEMENT MESH FOR 3-D LOCAL GEOSPHERE MODEL. ELEMENTS REPRESENTING THE VAULT ARE INDICATED BY THE DARK AREA IN THE CENTRAL PORTION OF THE MESH.

features in the conceptual model, and altered properties resulting from vault construction.

Transport Simulation

The calculation of radionuclide movement through the geosphere by solving the 3-D differential equations describing convection, diffusion, dispersion, chain decay and chemical retardation is very expensive.

As an initial step in transport modelling, particle tracking codes are being used to calculate radionuclide pathlines and travel times based only on groundwater velocity distributions predicted using MOTIF. Figure 12 illustrates travel predictions using the previously described 2-D flow analysis results. The path lengths from the vault to the surface do not vary a great deal, being two to three times the depth of the vault. However, the travel times in this simulation vary from 1200 years to 26 million years, the fastest path, D, being up the low-dipping fracture zone that intersects the vault.

The impact of thermal influences on convective transport is summarized in Table 1. The geothermal temperature gradient has minimal impact on path length but significantly reduces travel times. The vault heat also has a minimal influence on path length. The travel time along the fracture zone is somewhat reduced but there is minimal impact if a significant percentage of the path is through the rock mass.

These results indicate that a wide range of radionuclide transport scenarios may have to be considered. One extreme involves rapid convection in major fracture zones with transient thermal effects being important. In the other extreme convective transport through the bulk rock matrix may be negligible compared to diffusion, dispersion and retardation mechanisms. The relative importance is very sensitive to the proximity of major fracture zones to the vault.

To ensure adequate representation of diffusion and dispersion in the SYVAC submodel a detailed two-dimensional, finite-element, convective-dispersive transport model for the vault region is now being analysed using MOTIF. Preliminary results indicate a

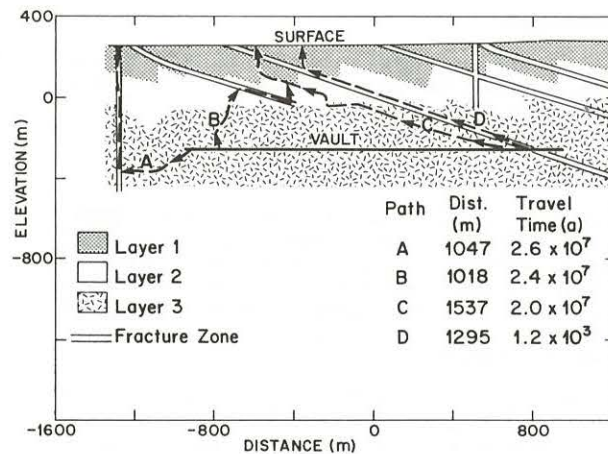


FIGURE 12: PREDICTED PATHS FOR CONVECTIVE TRANSPORT OF PARTICLES RELEASED FROM THE VAULT

rapid convection of contaminants up the low dipping fracture zone and then a significant dispersion in the near-surface layers. Dispersion and diffusion significantly accelerate the first arrival of contaminants along the slow paths but have only minor influence on transport along the faster paths.

CONCLUSION

Finite-element simulations of groundwater flow, conductive and convective heat transfer, and contaminant transport have been performed for a hypothetical geological disposal system in a very low-permeability rock mass traversed by a number of more permeable fracture zones. The results indicate that the fracture zones have predominant control over the migration of nonreactive contaminants from the vault to the biosphere.

TABLE 1: IMPACT OF GEOTHERMAL GRADIENT AND VAULT HEAT ON CONVECTIVE TRANSPORT

PATH	DISTANCE (m)		
	ISOTHERMAL	GEOTHERMAL	VAULT HEAT
A	1060	1040	1050
B	840	1020	1020
C	1530	1530	1540
D	1450	1450	1300

PATH	TRAVEL TIME (a)		
	ISOTHERMAL	GEOTHERMAL	VAULT HEAT
A	3.2×10^7	2.6×10^7	2.6×10^7
B	3.2×10^7	2.4×10^7	2.4×10^7
C	2.5×10^7	2.0×10^7	2.0×10^7
D	1.6×10^3	1.3×10^3	1.2×10^3

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