

Äspö Hard Rock Laboratory

Preliminary 2 km scale modelling of geochemical pathways Äspö HRL, Äspö Sweden

Task 5

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December 1998

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Keywords: Discrete fracture modelling, groundwater flow, solute transport, coupled hydrogeochemistry, pathways analysis, Äspö, Task 5

This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

ABSTRACT

This report describes preliminary modeling to demonstrate the application of FracMan Discrete Feature Network and PAWorks Pathways Analysis software to support Task 5, site scale hydro-geochemical modeling of the Äspö HRL site.

The modeling was carried out based on preliminary project data, and will be updated during 1999. The analysis defined the sources of water breaking through to the Äspö tunnel through pathways defined from a 2 km scale discrete fracture network model. Water sources are based on an initial spatial distribution of geochemical end-members, which makes it possible to calculate the geochemical end-member breakthrough to each point within the Äspö tunnel. The modeled period was from 1990 through 1996.

The analysis included development of a novel approach to incorporate the effect of varying density on flow velocity, based on a synthesis of the concepts of environmental and freshwater heads.

SAMMANFATTNING

Rapporten beskriver en preliminär modellering för att demonstrera tillämpningarna av programmen FracMan Discrete Feature Network och PAWorks Pathways Analysis inom Task 5, platsspecifik hydrogeologisk-hydrokemisk modellering av Äspölaboratoriet med omgivningar.

Modelleringen genomfördes baserat på preliminära projektdata och kommer att uppdateras under 1999. Analysen visar på ursprunget för vattnet som strömmar in till Äspötunneln med hjälp av flödesbanor identifierade i en diskret spricknätverksmodell i skalan 2 km. Vattnets ursprung baseras på en initial rumsligfördelning av ursprungsvattentyperna (med definerade grundvattenkemisk sammansättningar), vilket gör det möjligt att beräkna ursprungsvattens genomslag in till varje del av Äspötunneln. Modelleringperiod var från 1990 till 1996.

Analysen inkluderade en utveckling av en ny metod för att ta hänsyn till effekterna från densitetens påverkan på flödet, baserat på en syntes av koncepten för hydraulisk potential baserat på naturliga förhållanden (variabel densitetsfördening i vertikalled) och färskvattnen.

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Table 2-1 Structural Model Parameters

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EXECUTIVE SUMMARY

This report describes preliminary modeling to demonstrate the application of FracMan Discrete Feature Network and PAWorks Pathways Analysis software to support Task 5, site scale hydro-geochemical modeling of the Äspö HRL site.

The modeling was carried out based on preliminary project data, and will be updated during 1999. The analysis defined the sources of water breaking through to the Äspö tunnel through pathways defined from a 2 km scale discrete fracture network model. Water sources are based on an initial spatial distribution of geochemical end-members, which makes it possible to calculate the geochemical end-member breakthrough to each point within the Äspö tunnel. The modeled period was from 1990 through 1996.

The analysis included development of a novel approach to incorporate the effect of varying density on flow velocity, based on a synthesis of the concepts of environmental and fresh water heads.

1. INTRODUCTION

The aim of Task 5 of the Äspö Task Force on Modeling is to compare, and ultimately integrate, site scale hydrogeology and hydrochemistry by evaluating the large scale groundwater flow pathways activated by construction of the Äspö tunnels (Wikberg, 1998). This integration is expected to benefit underground radioactive waste repository performance assessment by providing a better understanding of transport pathways at the site scale.

The first stage in predicting this combined hydrogeological/geochemical response is to reproduce the chemical composition of the groundwater entering the Äspö tunnel. This is expressed as ratios of four geochemical "end-members," Meteoric, Glacial, Marine and Brine.

This report describes preliminary modeling to demonstrate the application of the FracMan Discrete Feature Network and the PAWorks Pathways Analysis Model to support Task 5. The goals of this modeling included:

- Develop a methodology to predict source locations for water recovered to Äspö tunnels
- Improve understanding of site scale transport pathways using geochemical information
- Incorporate the effect of varying density into the head solution used to compute the source location of flows into the tunnels
- Validate the PAWorks pathways analysis algorithms against in situ geochemical measurements

2. APPROACH

The JNC/Golder team approach to Task 5 is illustrated in Figure 2-1. The goal of initial modeling is to demonstrate the approach, based on initial data provided by SKB. Calibrated and predictive models will be developed during the next stage of this project during 1999.

2.1 PHYSICAL PROCESSES

The JNC/Golder team views Task 5 primarily within the context of site scale (2 km) solute transport pathways. These pathways which carry geochemical end-members to the Äspö drift can be thought of as analogues for the pathways for advective radionuclide transport from deep geological radioactive waste repositories. The processes considered in the analysis are as follows:

- a) laminar, variable density flow,
- b) identification of pathways,
- c) fluid storage in fracture pores, and
- d) advective transport in pathways

2.1.1 Laminar, Variable Density Flow

Using continuum principles of mass balance, the diffusivity equation which describes laminar flow can be written as (Bear, 1972):

$$\frac{\partial}{\partial x_i} \left[\frac{\mathbf{r}}{\mathbf{m}} k_{ij} \left(\frac{\partial P}{\partial x_i} + \mathbf{r}g \frac{\partial z}{\partial x_j} \right) \right] = \mathbf{r}(\mathbf{a} + \mathbf{fb}) \frac{\partial P}{\partial t} - q \quad (2-1)$$

where:

x_i	= coordinate directions (L)
ρ	= fluid density (M/L ³)
μ	= fluid viscosity (M/LT)
k_{ij}	= permeability (absolute) (L ²)
P	= fluid pressure (M/LT ²)
g	= gravitational acceleration (L/T ²)
z	= vertical direction (upward) (L)
α	= pore compressibility (LT ² /M)
ϕ	= porosity
β	= fluid compressibility (LT ² /M)
q	= source term (M/T)
t	= time (T)

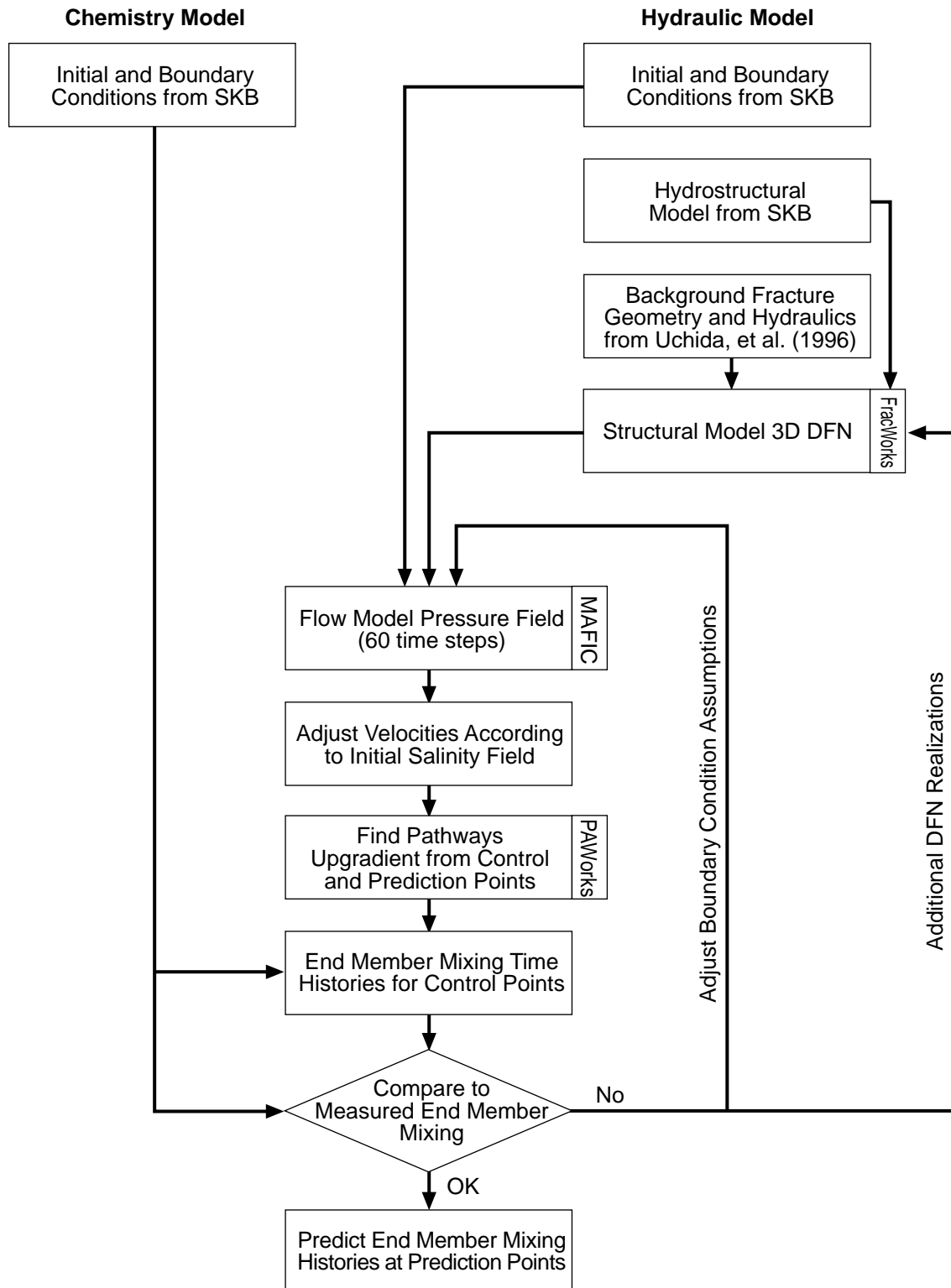


FIGURE 2-1
**FLOW CHART OF
 JNC/GOLDER APPROACH**
 PNC/TASK 5 REPORT/JAPAN

For a nearly incompressible fluid (e.g., water) flowing in two dimensions (e.g., in a fracture), the mass-conservation of Equation 2-1 can be simplified to a volume-conservation equation:

$$S \frac{\partial h}{\partial t} - T \nabla^2 h = q \quad (2-2)$$

where: S = Fracture Storativity (dimensionless)
h = Hydraulic head (L)
T = Fracture Transmissivity (L²/T)
q = Source/Sink Term (L/T)
t = Time (T)
∇² = Two-dimensional Laplace Operator

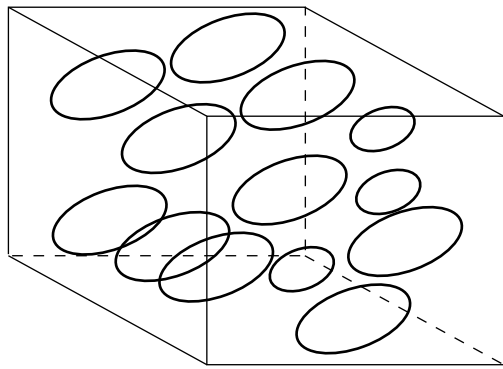
PAWorks solves the flow field using a finite element solution of Equation 2-2 for a network of rectangular pipes (Figure 2-2). In the current study, a steady-state flow solution was obtained for the pipe network to represent Äspö before tunnel construction, and a series of “snapshots” of the head field were obtained for a series of 60 transient boundary conditions reflecting weir fluxes due to tunnel construction. Each time step was equal to one month, with the head distribution at monthly intervals written to a file.

These pathways, head fields, and pipe properties were then post-processed to compute the pipe velocity in a variable-density system. In a variable-density flow system freshwater heads may be used to compute the head gradient along a horizontal plane, while environmental heads are accurate for computing vertical flow gradients. In these analyses the effect of increasing salinity with depth was included by correcting the finite element pipe velocities based on the freshwater and environmental head gradients, accounting for both flow direction and the relative density of the fluid in each pipe.

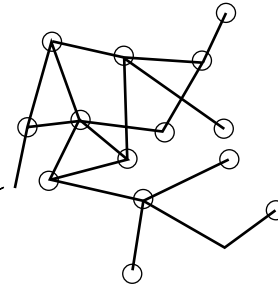
The environmental gradient $\Delta h^e / \ell_{ij}$ as a function of fluid density can be calculated as,

$$\frac{\Delta h^e}{\ell_{ij}} = \left[(h_i - h_j) \frac{\rho_w}{\rho_{ij}} + (z_i - z_j) \left(1 - \frac{\rho_w}{\rho_{ij}} \right) \right] / \ell_{ij} \quad (2-3)$$

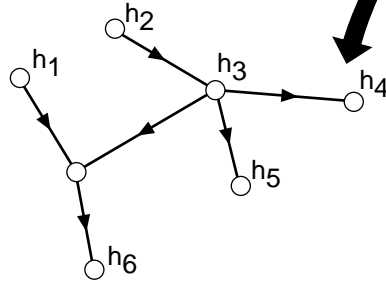
where h_i and h_j are freshwater head at the nodes i and j , ℓ_{ij} is the length of the pipe between nodes i and j , ρ_w and ρ_{ij} are the freshwater fluid density and the fluid density in the pipe between nodes i and j , and z_i and z_j are the elevations of nodes i and j .



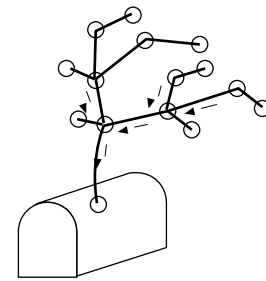
Realistic fracture pattern



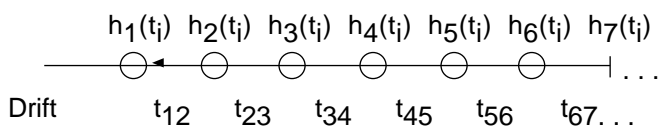
3D pipe connectivity topology



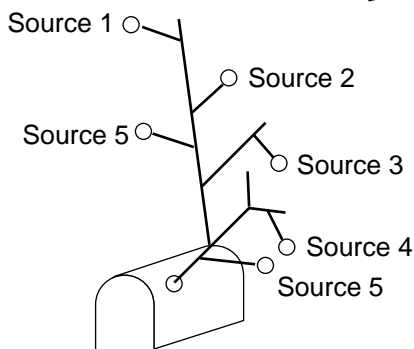
Finite element flow solution defines heads and flows in network (60 timesteps)



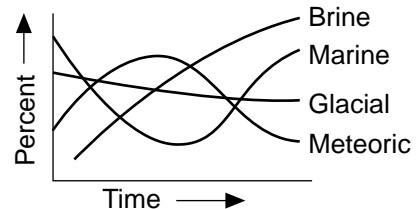
Search through network following flux upgradient from drifts



Calculate density adjusted travel times along pathways for segment jk during time step i



Calculate source for water arriving at drift during each timestep based on density adjusted travel times



Match source locations to initial end member distributions to calculate end member breakthrough to drift locations

FIGURE 2-2
PAWorks PIPE
NETWORK APPROACH
PNC/TASK 5 REPORT/JAPAN

Velocity-based freshwater and environmental heads are derived by interpolating a function of the orientation of the pipe dip ϕ , on $[-\pi/2, +\pi/2]$ where $-\pi/2$ represents upward flow, 0° represents horizontal flow, and $+\pi/2$ represents downward flow. The relative velocity v_{ij}/v_o is,

$$\frac{v_{ij}}{v_o} = \left(\cos^2 \mathbf{f} + \sin^2 \mathbf{f} \left(\frac{\mathbf{r}_w}{\mathbf{r}_{ij}} + \frac{\ell_{ij}}{h_i - h_j} \sin \mathbf{f} \left(1 - \frac{\mathbf{r}_w}{\mathbf{r}_{ij}} \right) \right)^2 \right)^{1/2} \quad (2-4)$$

Density is related to chloride Cl^- as total dissolved solids (TDS),

$$\mathbf{r}_{ij} = \mathbf{r}_w + \text{TDS} \times 10^{-6} \quad (2-5)$$

where ρ_w is 0.9997 g/ml and TDS is expressed as (mg/l).

The velocity variation with pipe orientation for a relative density of 1.05 is shown in Figure 2-3. Figure 2-3 illustrates how the velocity relative to the freshwater simulation decreases for upward flow, increases for downward flow, and is unaffected for horizontal flow. The variation of velocity with increasing density is shown in Figures 2-4 and 2-5, for vertically upward and downward flow, respectively.

The density profile for this simulation was based on chemistry data from regional boreholes (Rhen, 1998). Figure 2-6 illustrates the variation in fluid density for seven deep Äspö boreholes. The regression shown in Figure 2-6 excludes data from KLX002, which shows fresh water at depths of over 800 meters.

2.1.2 Pathway Identification

Pathways are identified up-gradient from each of the calibration points and prediction points in the tunnel (Figure 2-7). These pathways are identified by searching up-gradient from these points, based on the head distribution following construction of the tunnel to 3600 m. Pathway search identifies every node up-gradient, from the calibration and prediction points to the boundary conditions.

These pathways represent the potential sources for the geochemical end-members produced in the tunnels. A depth-first, flux-weighted search is used, which means that the code preferentially follows the higher flow pathways. In the current analysis, the search was limited to finding only twenty pathways per source fracture representing the tunnel calibration and prediction points.

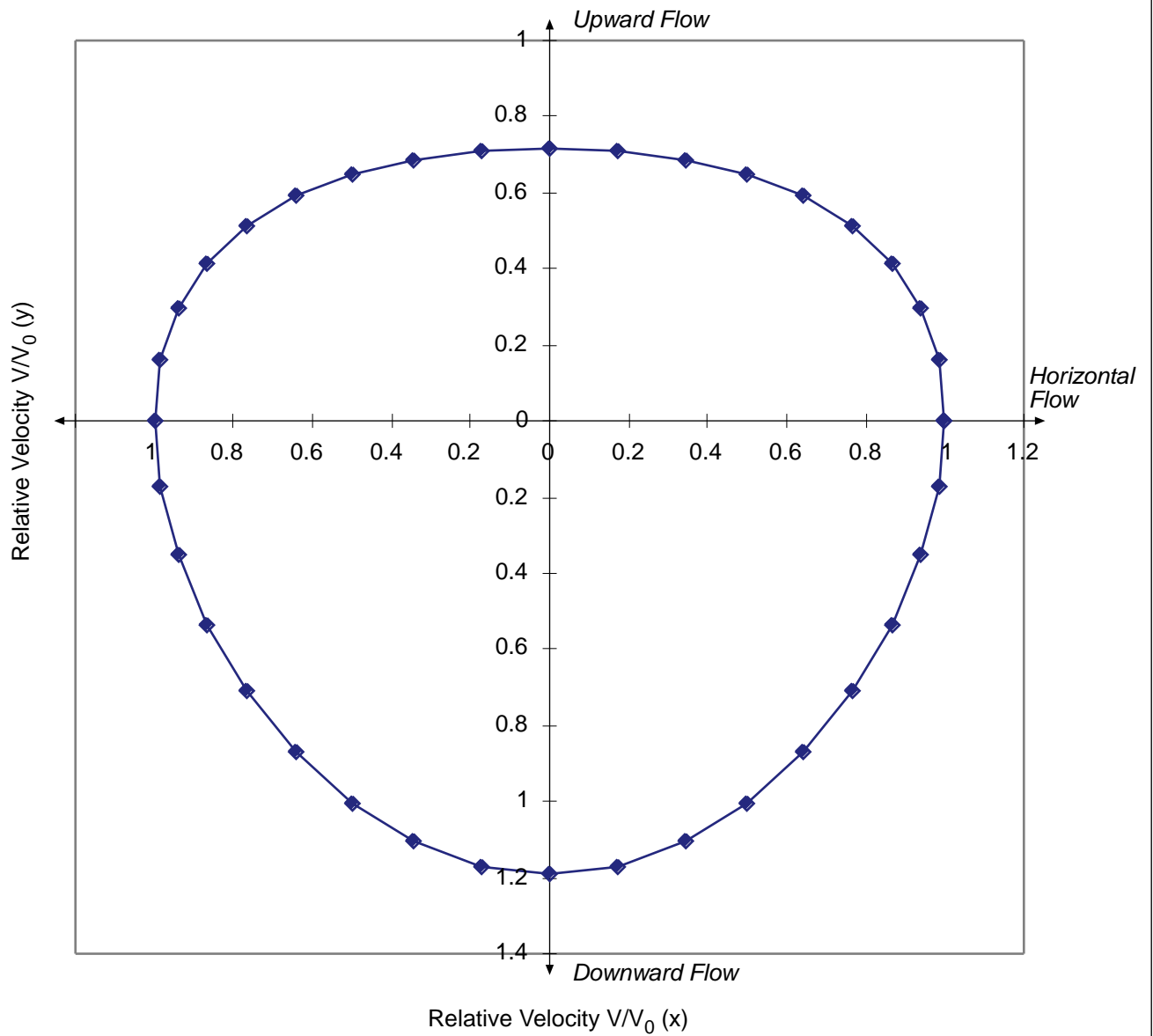


FIGURE 2-3
 RELATIVE VELOCITY V/V_0
 VERSUS DIP ϕ OF PIPE
 PNC/TASK 5 REPORT/JAPAN

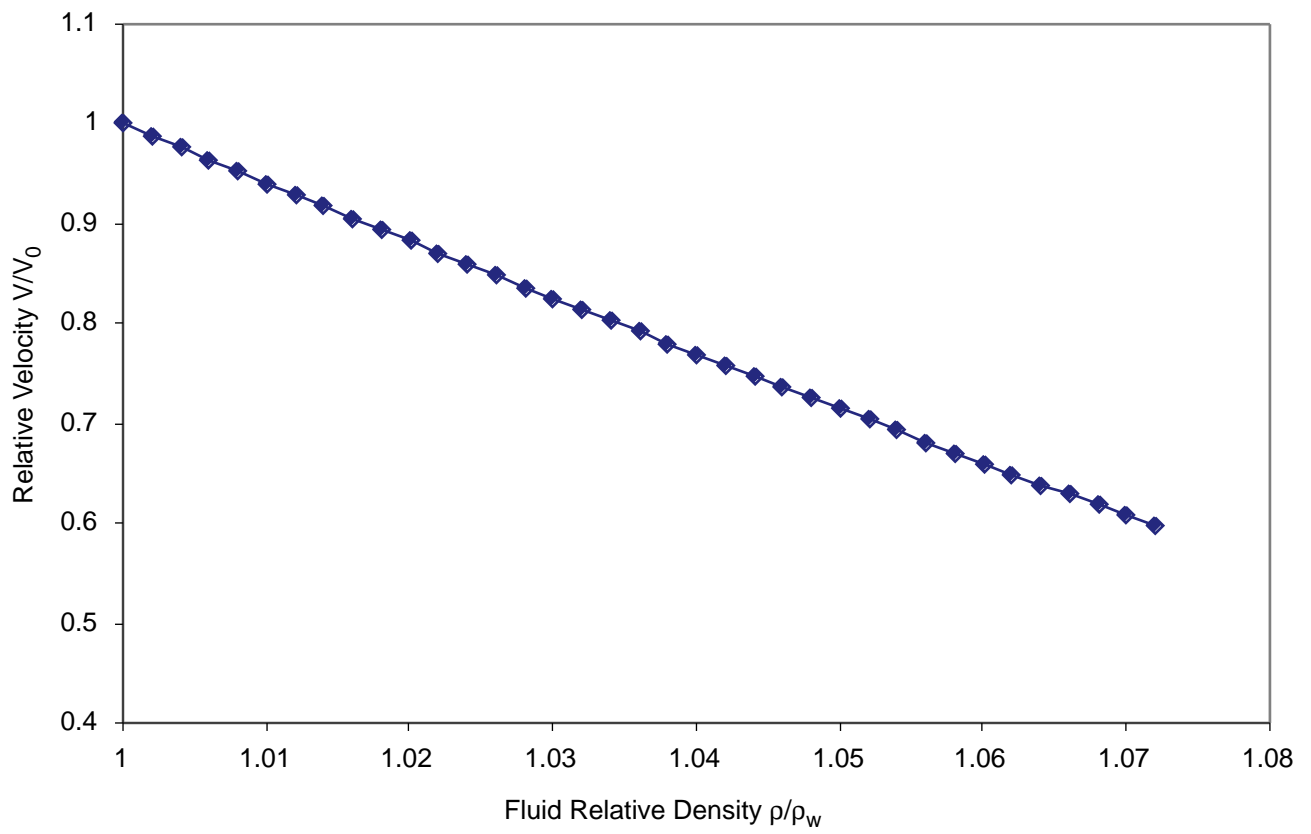


FIGURE **2-4**
RELATIVE VELOCITY V/V_0 FOR
VERTICALLY UPWARD FLOW
 PNC/TASK 5 REPORT/JAPAN

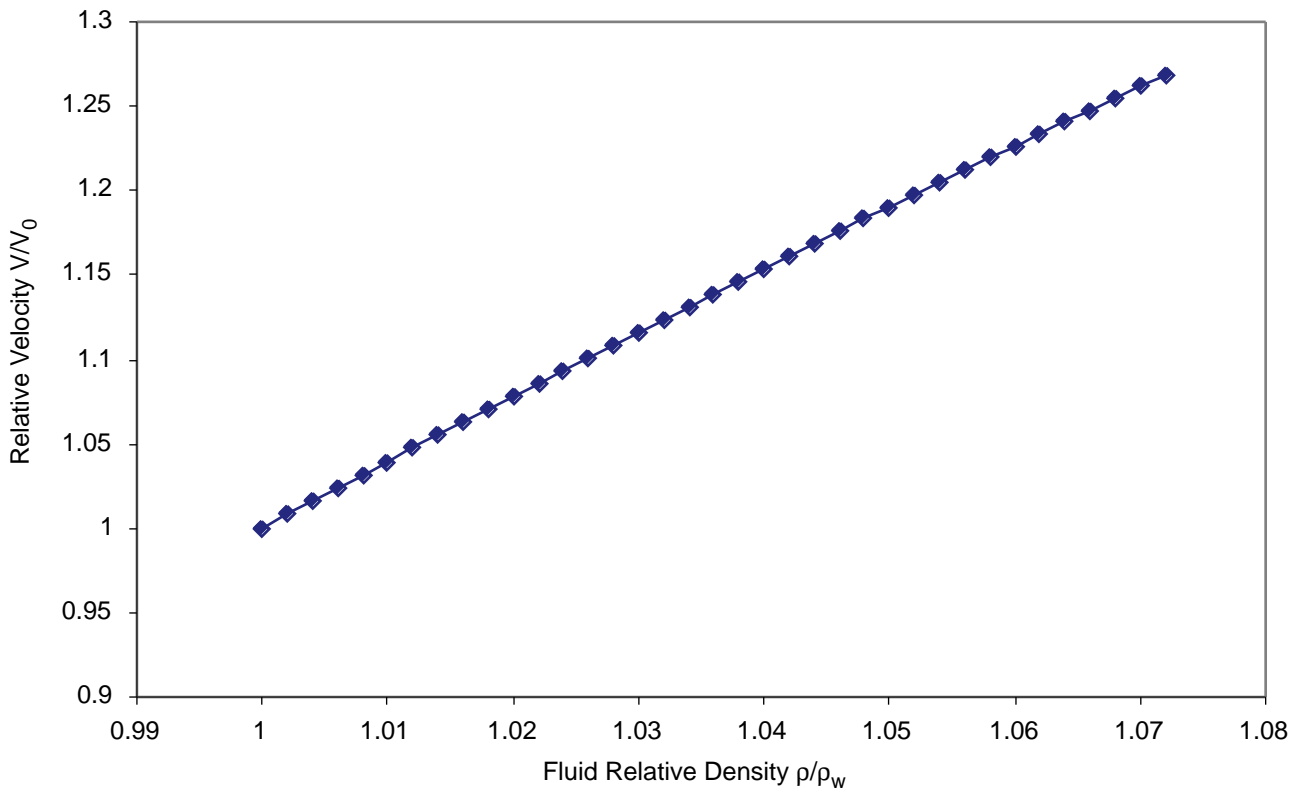
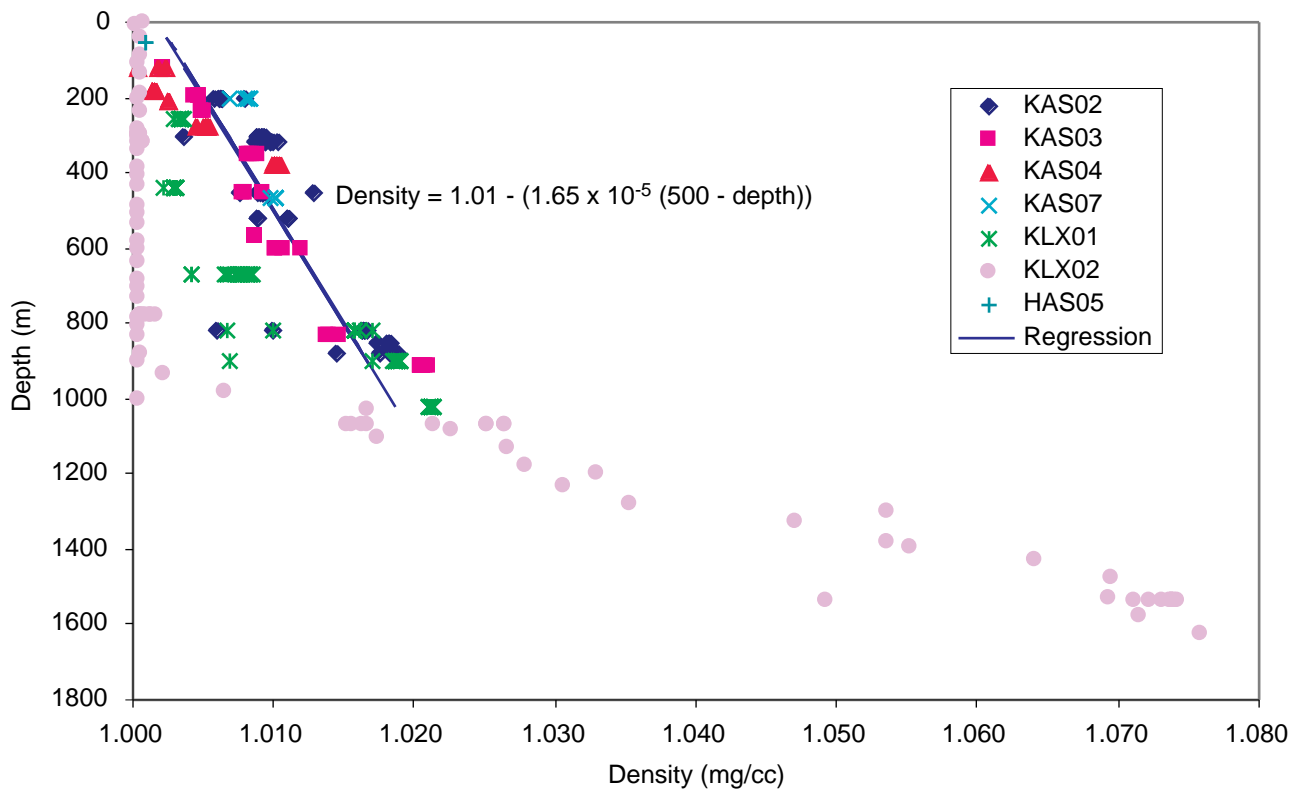
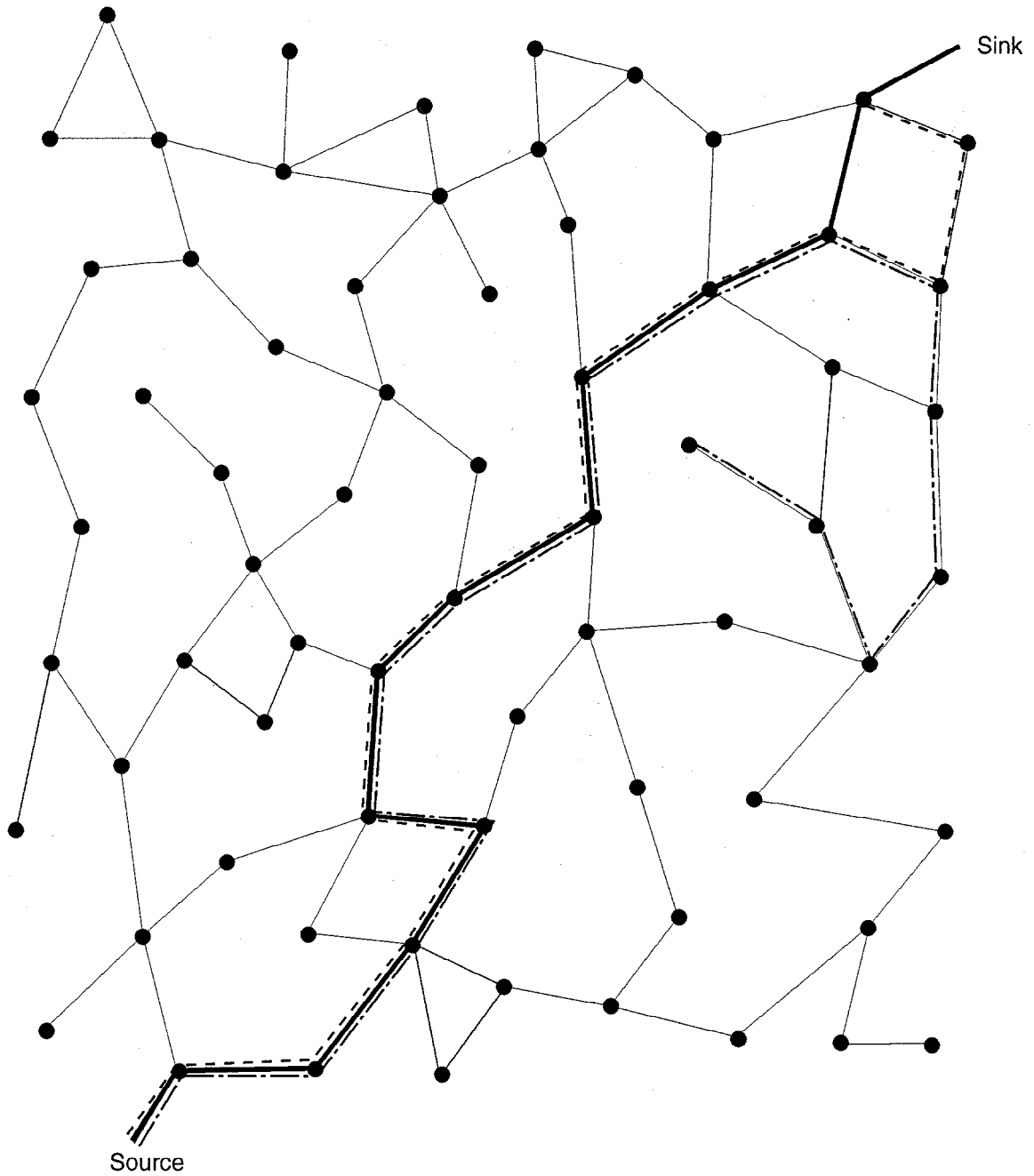


FIGURE **2-5**
RELATIVE VELOCITY V/V_0 FOR
VERTICALLY DOWNWARD FLOW
 PNC/TASK 5 REPORT/JAPAN



Regression does not include KLX02

FIGURE 2-6
**FLUID DENSITY FROM
 ÄSPÖ BOREHOLES**
 PNC/TASK 5 REPORT/JAPAN



- First Iteration: path found
- - - Second Iteration: path found
- · - · - Third iteration: path not found

FIGURE **2-7**
PATHWAY SEARCH UPGRADIENT
PNC/TASK 5 REPORT/JAPAN

Sixty “snapshots” of the head field in the pipe network were used to define the pathways for flux to the tunnel sections. For each head field time step, a PAWorks pathways analysis was carried out for each tunnel section to identify the source of the water arriving in the tunnel during that time step, using density-corrected velocities. Velocities were calculated for each time step, and the distance traveled along each pathway during a time step is calculated using this velocity.

2.1.3 Fluid Storage Porosity

Most end-members produced in the tunnels are assumed to come from storage within the rock mass. Therefore, the amount of fluid stored in the rock mass is a key to the geochemical predictions and pathways. In the current analysis, the total volume of fluid storage in all fractures was represented as 100 times the fracture storativity for the fractures in the upgradient pathways. This represents an assumption that only approximately 1% of conductive fractures are included in the model. Based on this assumption, fracture storativity S is related to fracture transmissivity T as,

$$S = 0.1 T^{1/2} \quad (2-6)$$

Based on Equation 2-6, storativity for major fracture zones ranges from 3×10^{-3} to 3×10^{-4} for fractures of transmissivity 10^{-3} to 10^{-5} m²/s.

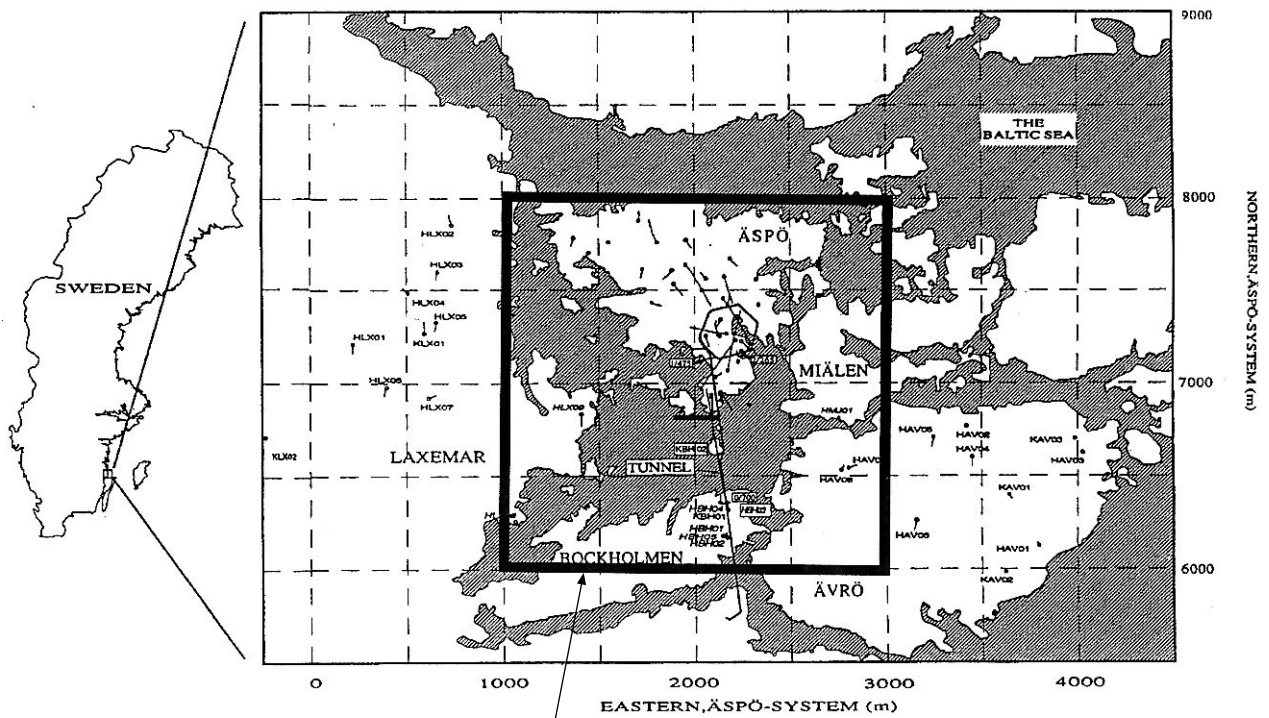
2.1.4 Advective Transport and Mixing

Geochemical end-members are assumed to be transported to the calibration and prediction points solely by advection along defined pathways. Complete mixing is assumed at all pipe intersections.

2.2 STRUCTURAL MODEL AND MATERIAL PROPERTIES

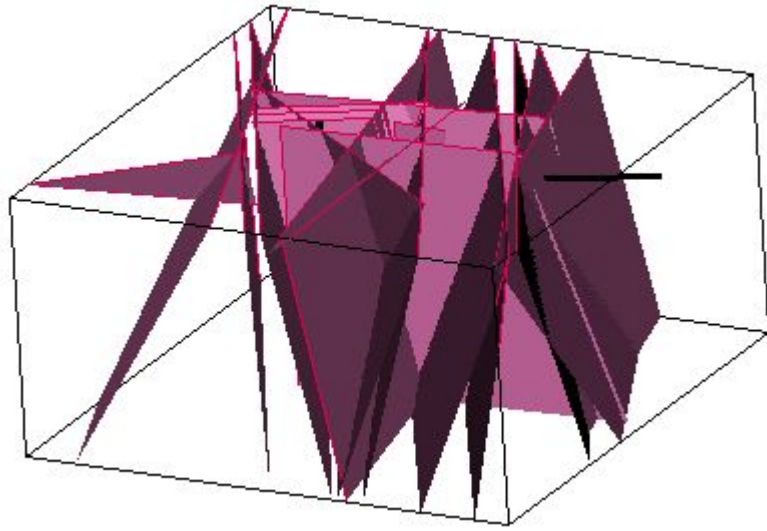
The region modeled was 2000 m by 2000 m in area, with a depth of 1000 m (Figure 2-8). This scale was selected to include the Äspö tunnels and extend the boundaries as far as possible given computation time constraints.

The structural model used for these analyses is based on the DFN approach, in which all fluid storage, flow, and transport occurs through a limited subset of “conductive structures” represented by polygonal plates. The structural model is described in SKB ICR 97-03 (Uchida et al., 1997). The model is illustrated in Figure 2-9 and summarized in Table 2-1. For the purposes of this demonstration only the 22 deterministic fractures zones and the stochastic background fractures were included. These fracture sets are shown in Figures 2-9a and 2-9b respectively. The derivation of this model is explained in Uchida et al, 1997.

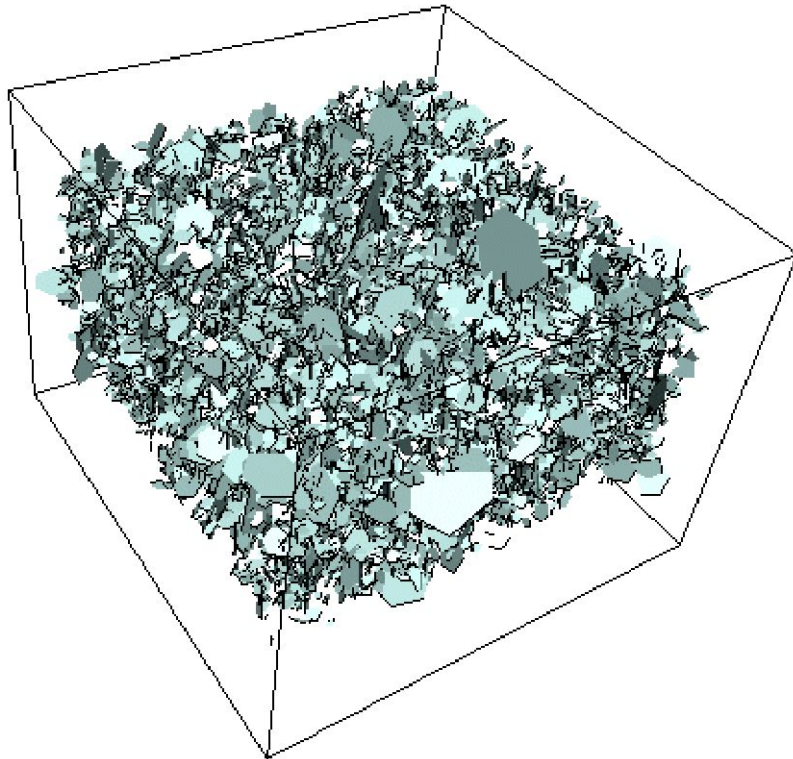


**Modeled Region for
Preliminary Task 5
Simulations**

FIGURE 2-8
ÄSPÖ TASK 5 MODELING REGION
PNC/TASK 5 REPORT/JAPAN



a. Fracture Zone Features



b. Background Fractures

Table 2-1 Structural Model Parameters

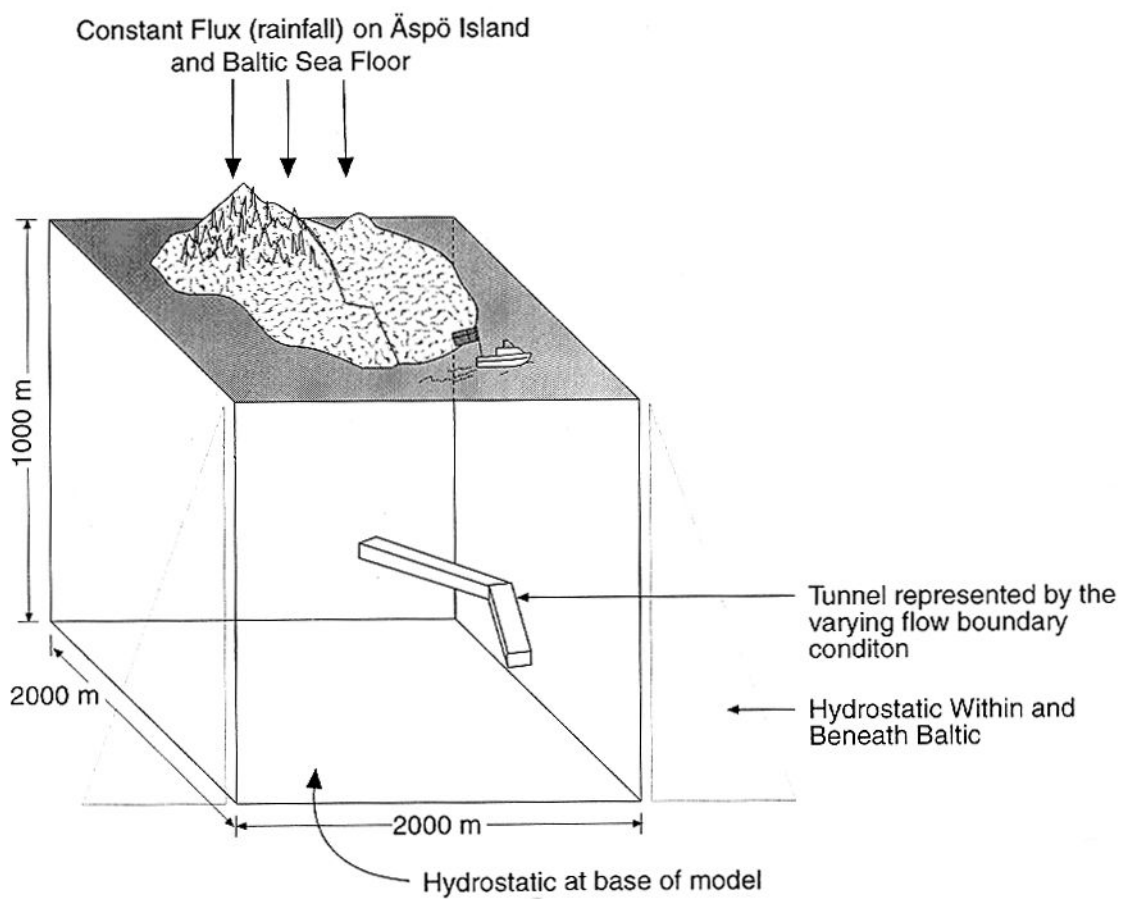
Fracture Set	Deterministic Fracture Zones	Background Fracture Properties
Name	Fracture Zone Fractures	Background fractures
Location	22 Planar Homogeneous Zones	Baecher/Bart Model
Size	Surface Traces Mean = 1420 m	LogNormal ($\mu = 13.7$ m, $\sigma = 12.7$ m)
Orientation	3 Point Solution	Bootstrap SKB, 1994 Fractures Mapped in Tunnels
Transmissivity	TR-91-22 & Olsson, 1995a	LogNormal ($\mu = 9 \times 10^{-7}$ m ² /s, $\sigma = 5 \times 10^{-6}$ m ² /s)
Storativity	0.001 T ^{1/2}	0.001 T ^{1/2}
Intensity	Surface traces P ₂₁ = 7.83 x 10 ⁻³ (m/m ²)	P ₃₂ = 0.020214 (m ² /m ³)

2.3 BOUNDARY AND INITIAL CONDITIONS

Simplified boundary conditions of the model were used for these preliminary simulations and are shown in Figure 2-10. The base and sides of the model were modeled as hydrostatic. The surface of the model was modeled with a constant infiltration rate of 7.5 mm/year, equivalent to precipitation of 30 mm/year over Äspö Island.

The simulation covered the construction of the tunnels between July 1, 1991 and 16 January, 1994, with the flows extrapolated to June 4, 1996. Within PAWorks, the Äspö tunnels were treated as time-varying group flux boundary conditions. Therefore, for any individual section of tunnel, prior to its construction it had a net flux of zero; after construction its flux was equal to the measured flow into that tunnel section from weir data to 2900 m.

For the predictive portion of the tunnels (2900 m to 3600 m), it was assumed that flux from weirs to 2900 m would maintain constant flux, and that weirs MA2994G and MA3179G would produce 4.4×10^{-4} m³/s and 2.5×10^{-4} m³/s respectively, consistent with production rates per meter of weir MA2840G. The total flux to the drifts as a function of time is illustrated in Figure 2-11. Figure 2-12 summarizes the distribution of five geochemical end-members included in initial SKB data distributions with depth, for sampling points under land. Figure 2-13 illustrates the density distribution with depth, assuming reference densities for each of the geochemical end-members.



Schematic- Not to scale

FIGURE **2-10**
BOUNDARY CONDITIONS
PNC/TASK 5 REPORT/JAPAN

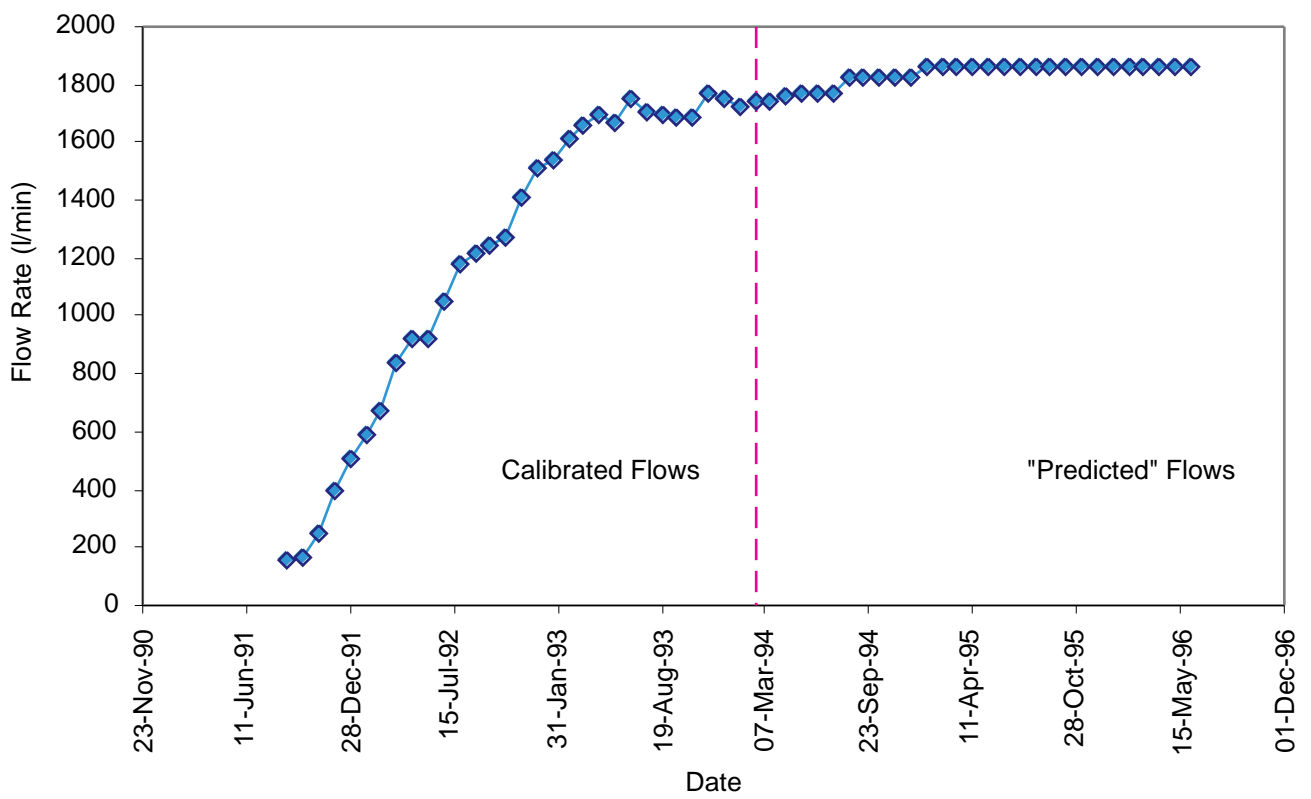


FIGURE **2-11**
WEIR FLUX TO JUNE 4, 1996
 PNC/TASK 5 REPORT/JAPAN

Water Chemistry with Depth - Under Land

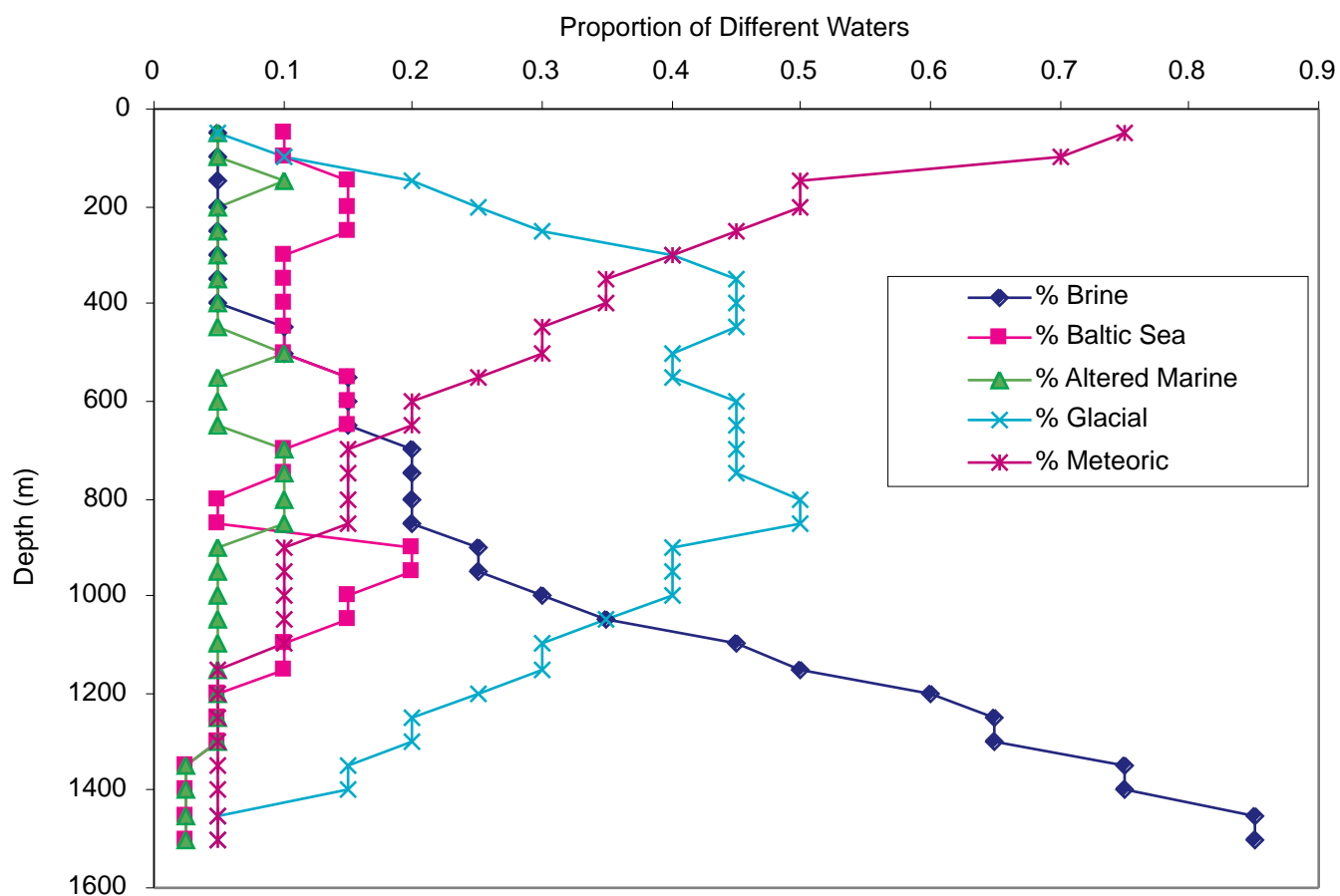


FIGURE 2-12
 END MEMBER DISTRIBUTION WITH DEPTH
 PNC/TASK 5 REPORT/JAPAN

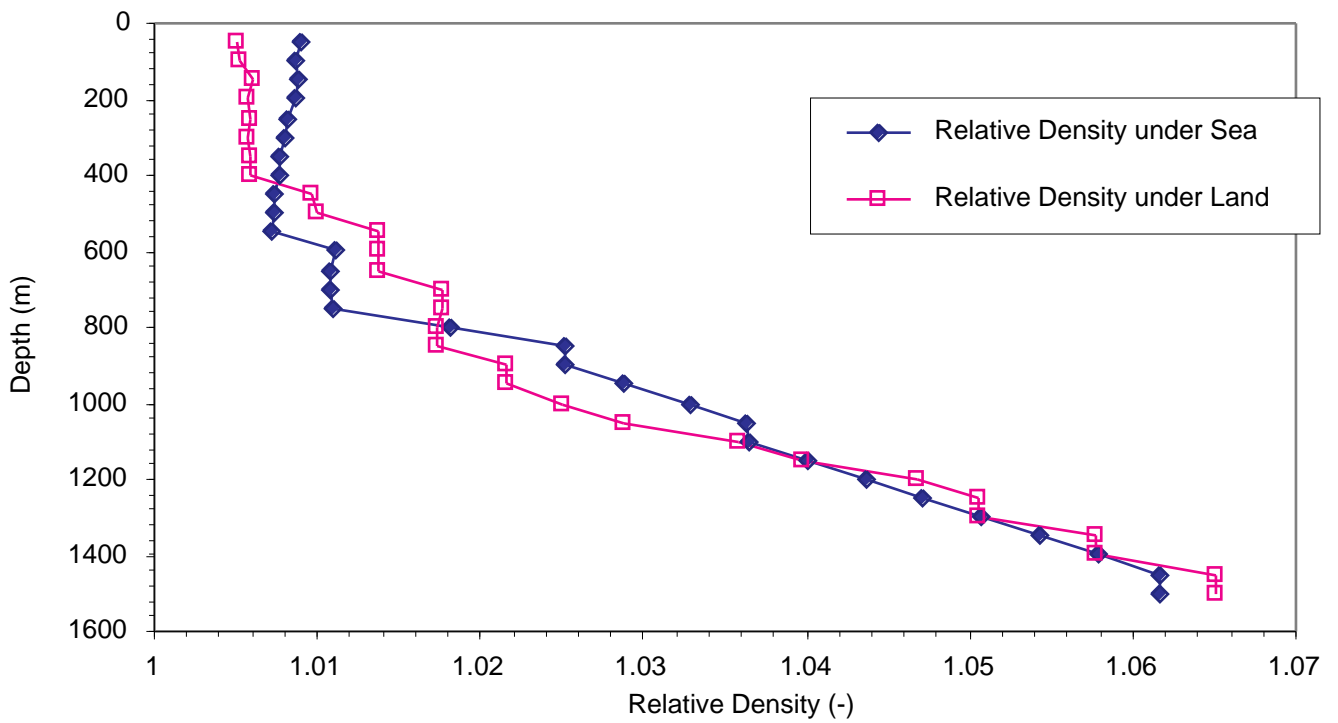


FIGURE **2-13**
DENSITY DISTRIBUTION WITH DEPTH
 PNC/TASK 5 REPORT/JAPAN

The initial conditions for the geochemical end-members were obtained by using linear or non-linear interpolation to approximations to the geochemical end-member measurements provided by SKB (Rhen, 1998). The equations for calculation of the initial end-member mix as a function of geochemical end-member initial condition measurements and the data used are illustrated in Figures 2-14a (glacial), 2-14b (meteoric), 2-14c (marine), and 2-14d (brine).

2.4 SOFTWARE

The FracMan discrete feature network model was used for this analysis. In particular, FracMan/FracWorks was used for generation of background discrete fractures, FracMan/MAFIC was used for steady state and transient flow simulations, and FracMan/PAWorks pathway analysis was used to define pathways. FracMan is described in Appendix A of SKB 97-03 (Uchida et al, 1997) and in more detail in the FracMan manual (Dershowitz et al., 1998a), MAFIC manual (Miller et al., 1998) and PAWorks manual (Dershowitz et al., 1998b).

FracMan/PAWorks is a suite of analysis codes which represent fracture networks as a 3-D pipe network, with nodes defined by fracture intersection traces. The advantage of using pipe elements, as opposed to plate elements, is that there is a vast saving in memory and computation time requirements. In PAWorks, the pipes are generated to maintain the connectivity structure of the 3-D discrete fracture network, with approximately equivalent conductances and surface areas (Figure 2-15).

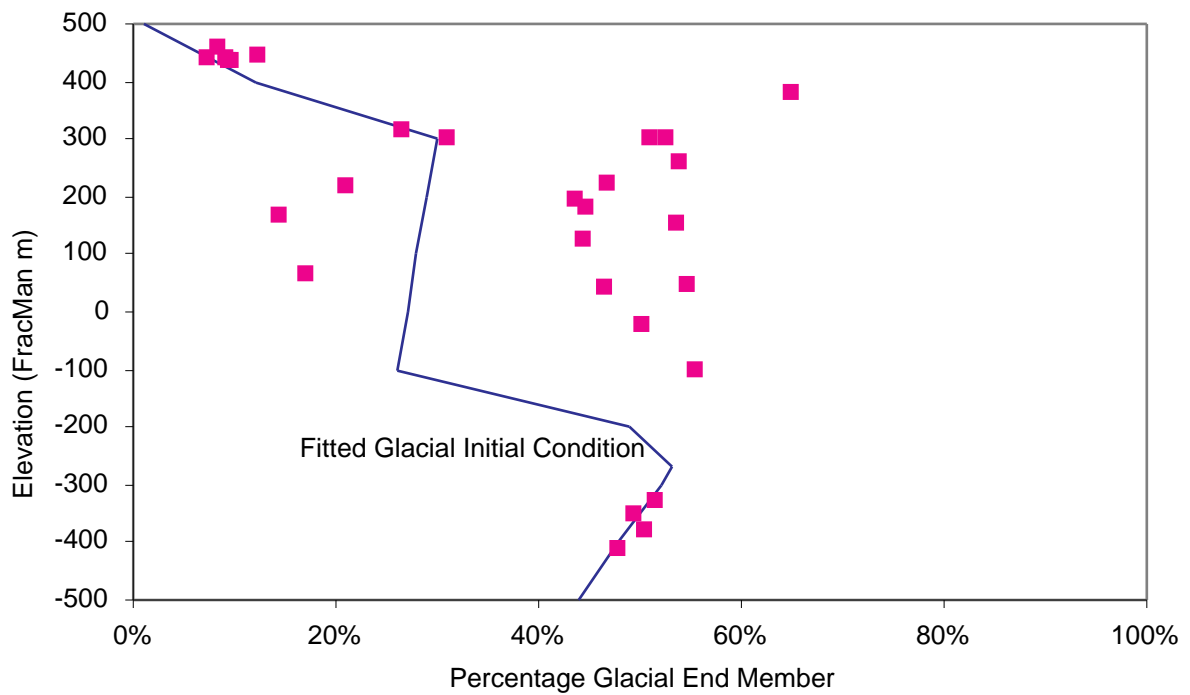


FIGURE **2-14a**
GLACIAL END MEMBER
INITIAL CONDITION
 PNC/TASK 5 REPORT/JAPAN

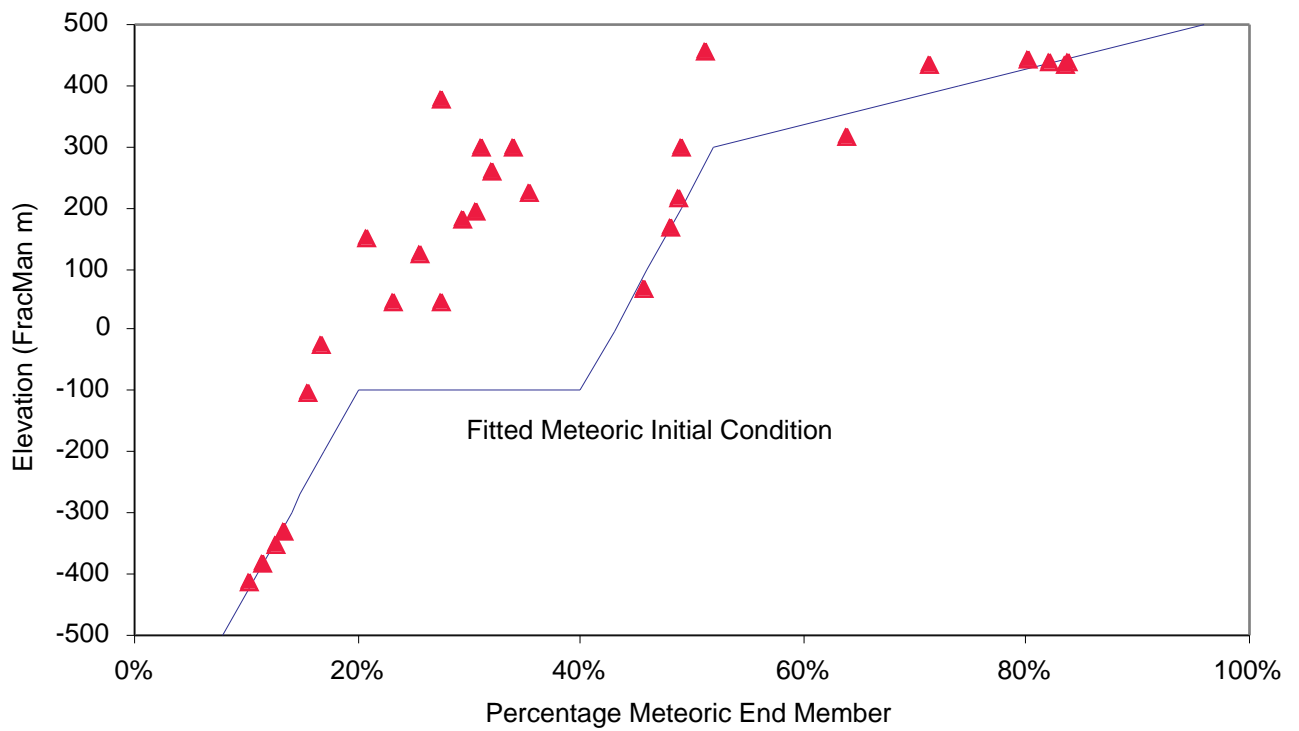


FIGURE **2-14b**
METEORIC END MEMBER
INITIAL CONDITION
 PNC/TASK 5 REPORT/JAPAN

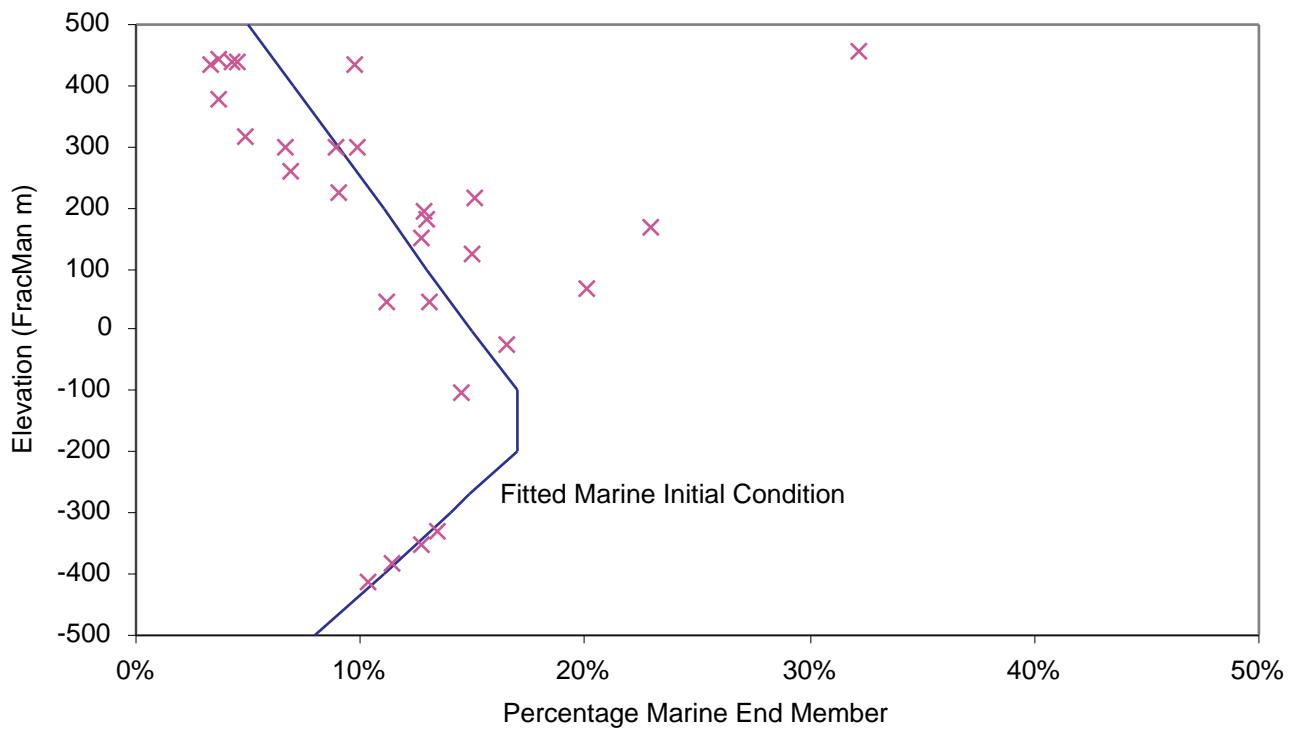


FIGURE **2-14c**
MARINE END MEMBER
INITIAL CONDITION
 PNC/TASK 5 REPORT/JAPAN

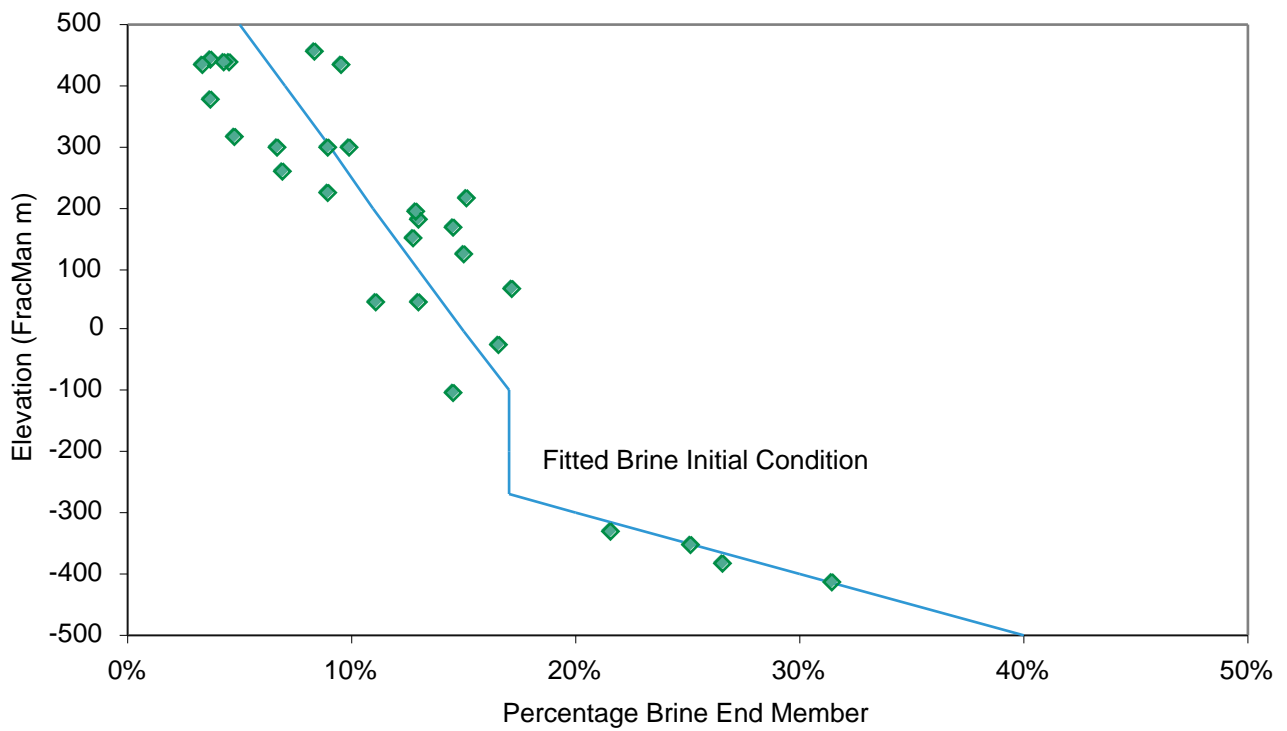
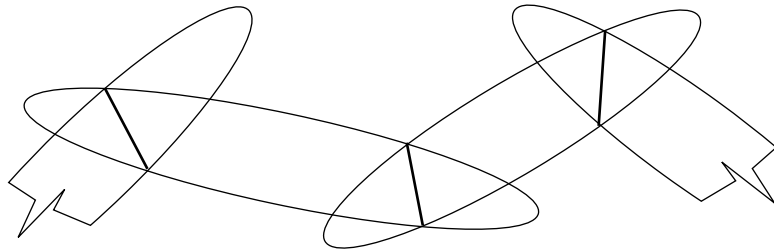
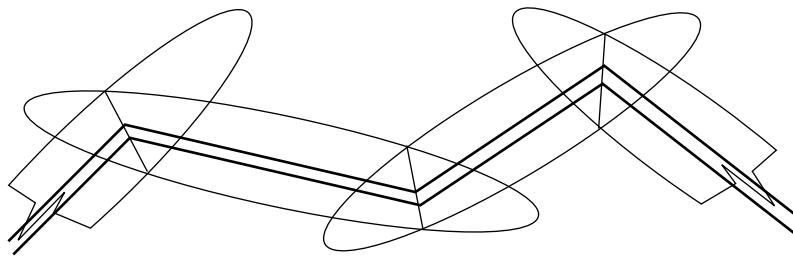


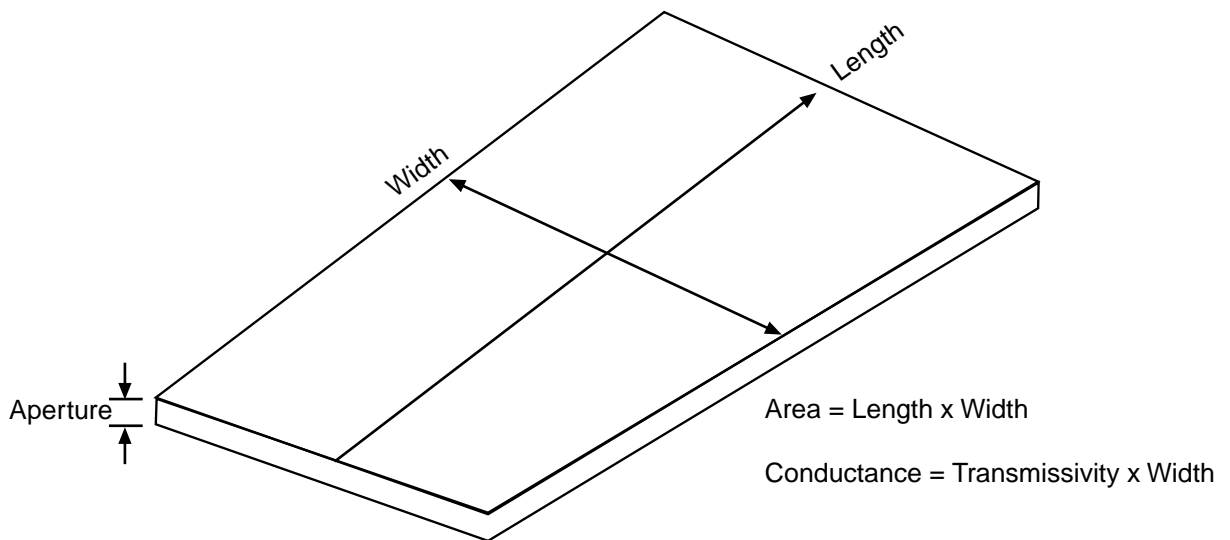
FIGURE **2-14d**
BRINE END MEMBER
INITIAL CONDITION
 PNC/TASK 5 REPORT/JAPAN



Step 1: Calculate Intersections



Step 2: Define Pipes



Step 3: Calculate Pipe Properties

FIGURE **2-15**
PAWorks PIPE NETWORKS
FROM FRACTURES
 PNC/TASK 5 REPORT/JAPAN

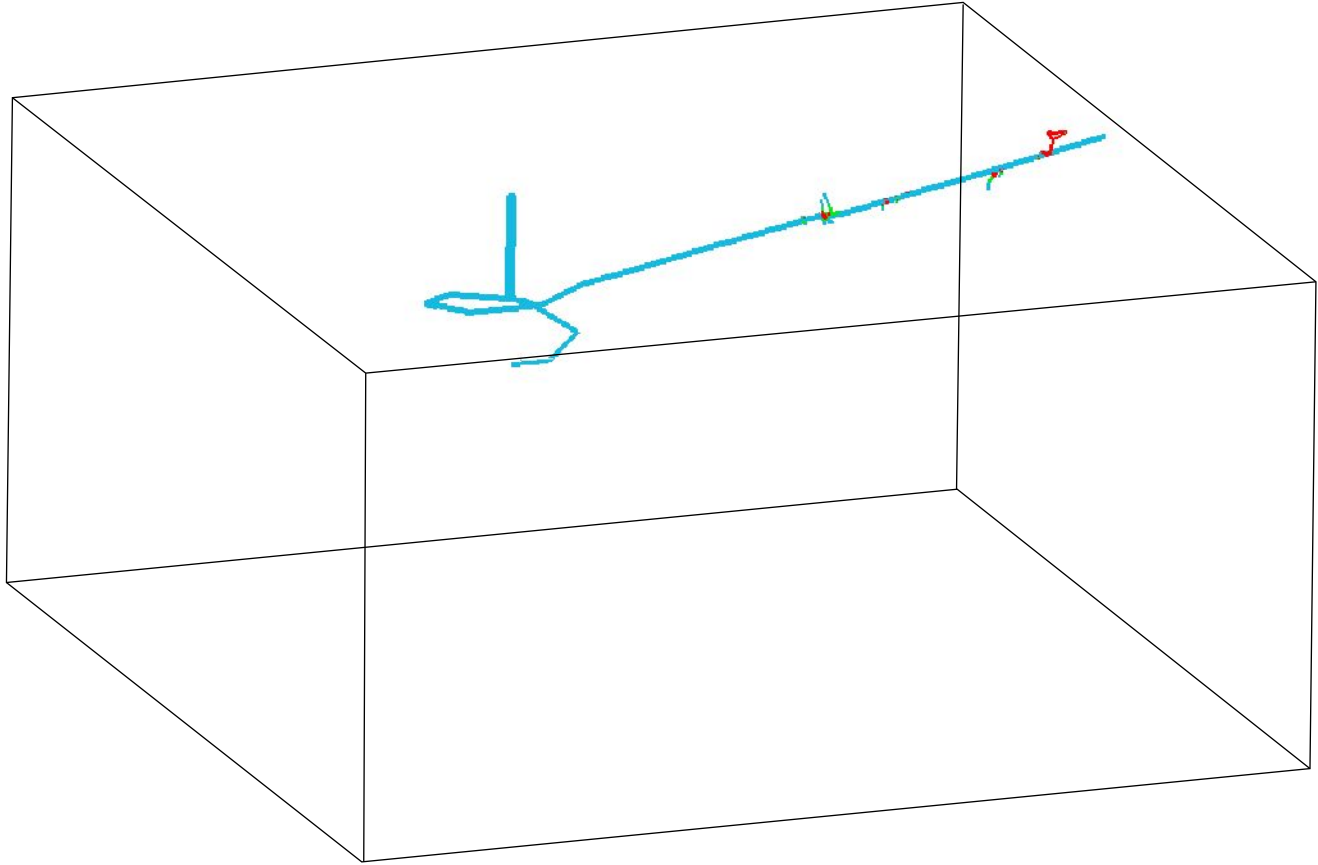
3. PRELIMINARY SIMULATIONS

The PAWorks analysis provides results as the source locations of the water flowing into the tunnels on a monthly basis. These locations have been shown as plots of the source location of the water flowing into the tunnels on a monthly basis. Figures 3-1 through 3-8 illustrate the source locations for waters produced to the drift during the first 24 months of construction. These figures are based on preliminary simulations without velocity corrections for density.

The simulations indicate that initially all the water flowing into the tunnel is located very close to the tunnel, which is to be expected. With time, the source of water flowing into a small section of tunnel may have originated from quite different sections of the fracture network, and are poorly correlated to the Cartesian distance from the tunnel. In particular, at later times and close to the shaft locations (see Figure 3-8) there are an extremely wide range of water source locations. This may be influenced both by the duration of extraction at the earlier constructed tunnel sections and the complexity of the boundary condition in the vicinity of the shafts.

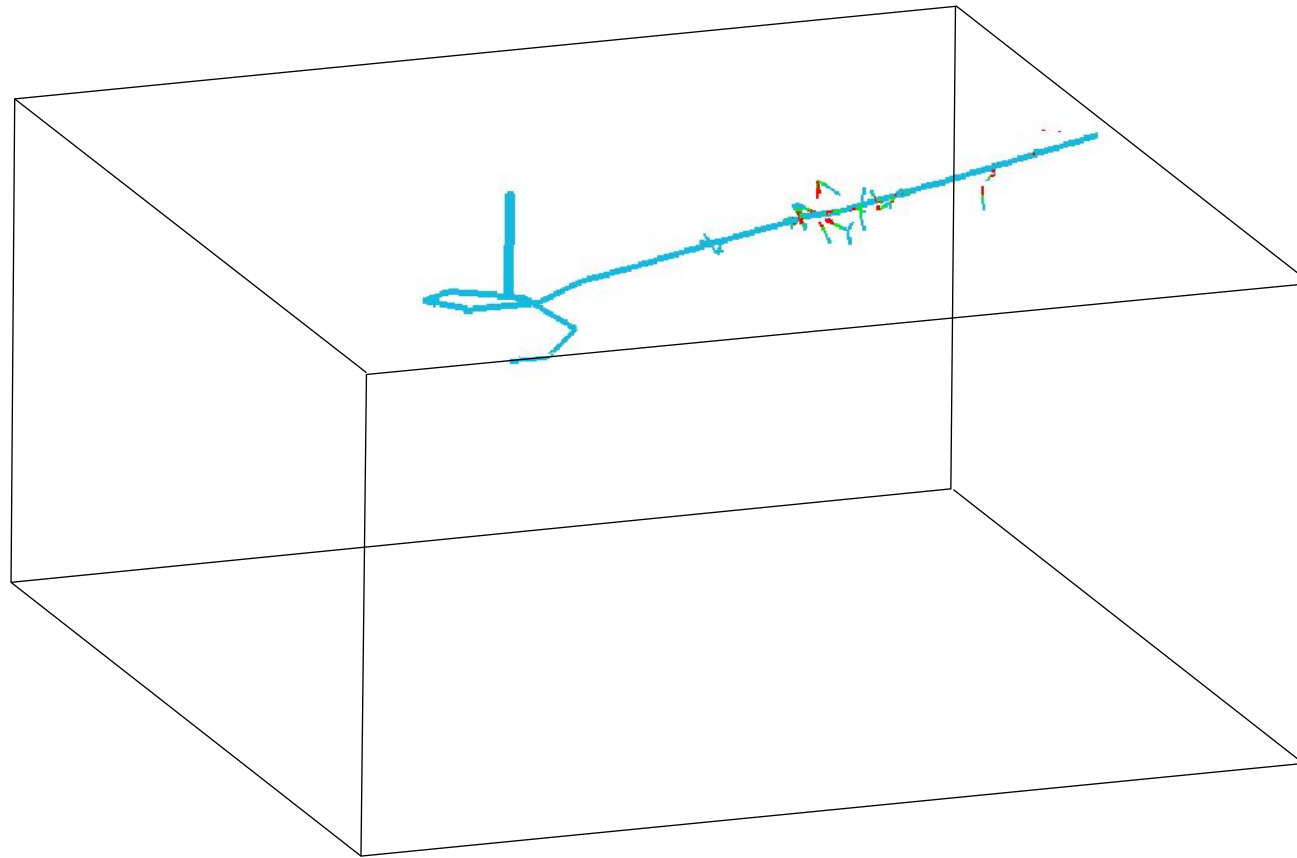
In our preliminary model there is a preferential bias to upwards vertical flow from beneath the tunnel. This result seems generally consistent with the chloride measured during tunnel construction. However, while the results are interesting, at this stage in the modeling sensitivity to boundary conditions has not yet been investigated and it is too early to draw firm conclusions.

Figures 3-9 through 3-12 present example geochemical end-member mix breakthrough to preliminary control points for simulations including the velocity correction for density effects. These results indicate that the current model does not provide for sufficient recharge from the Baltic boundary condition, but is able to match many of the general geochemical trends observed.



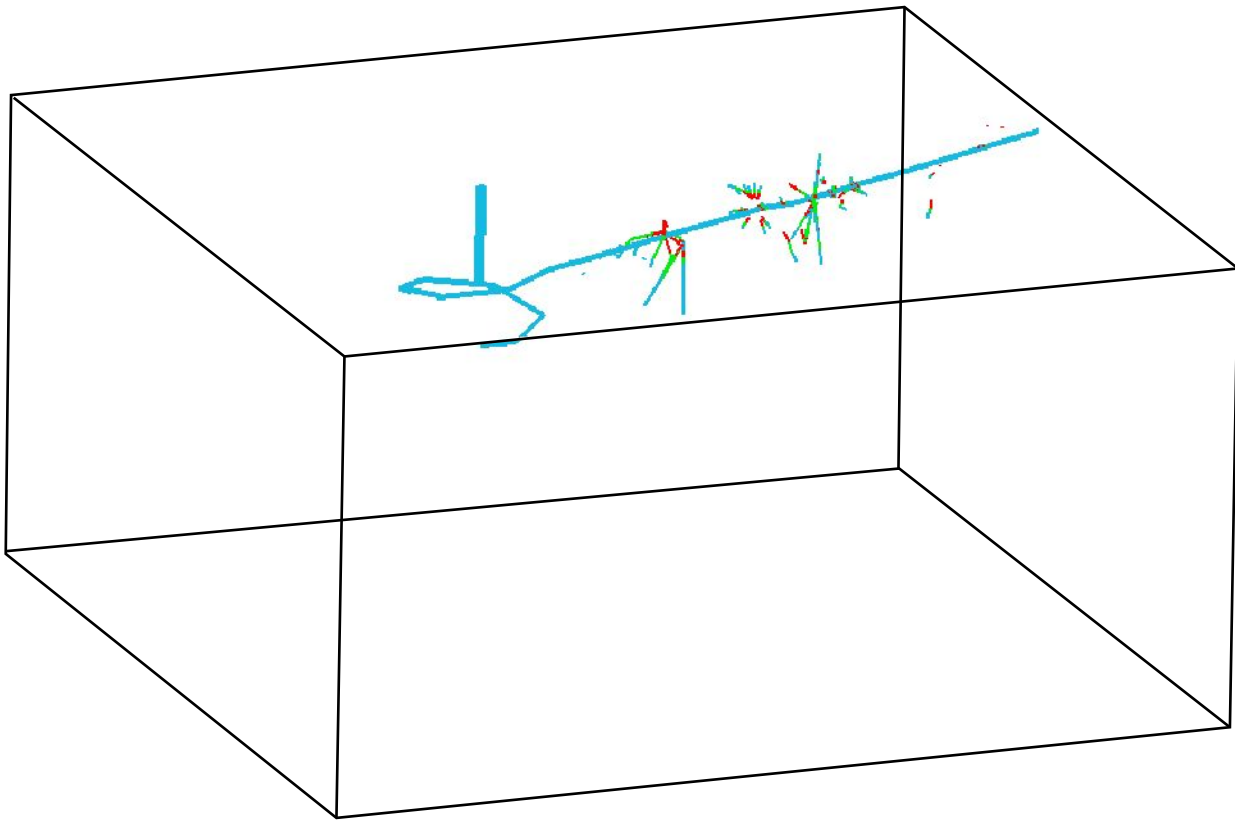
- 0-1 months
- 1-2 months
- 2-3 months

FIGURE **3-1**
**SOURCE LOCATION OF WATER
IN TUNNELS, 0-3 MONTHS**
PNC/TASK 5 REPORT/JAPAN



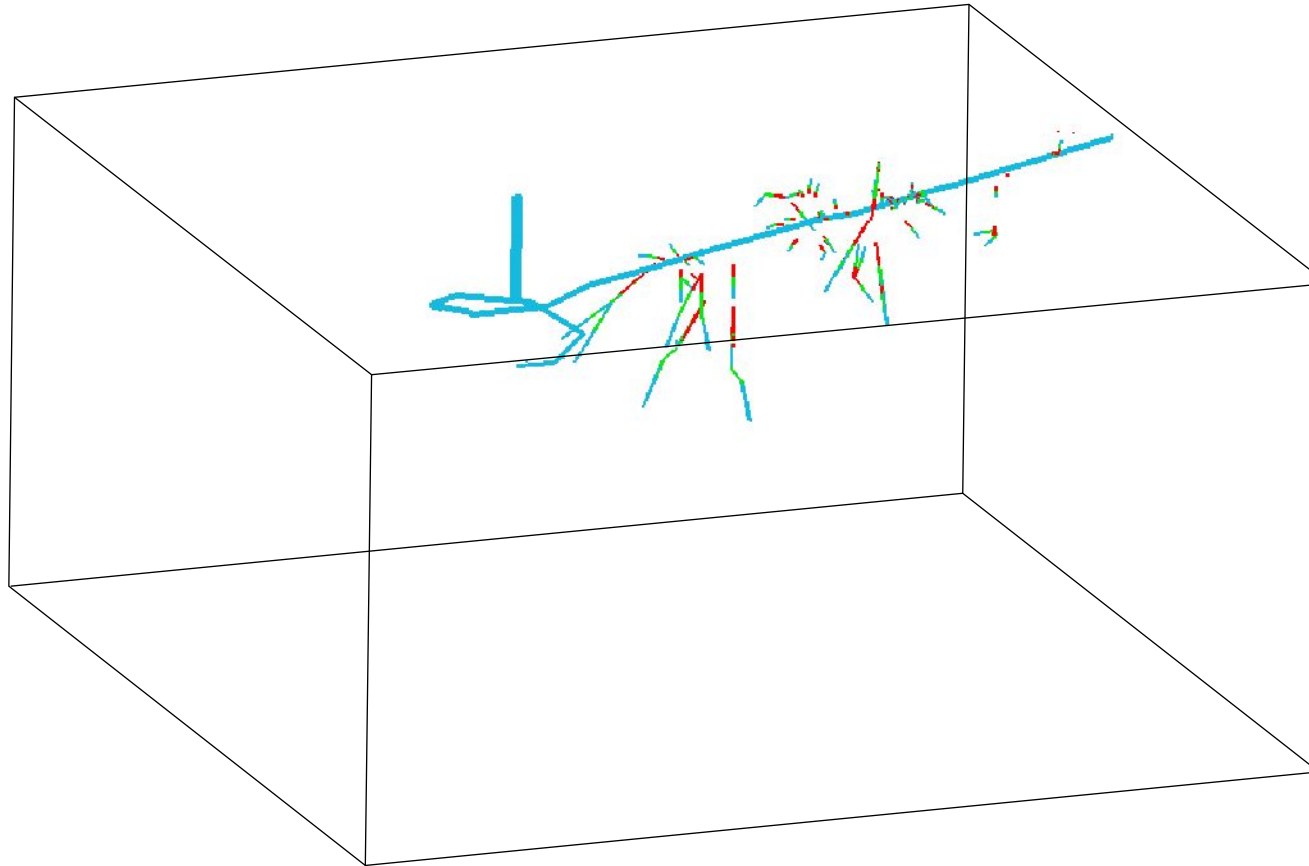
- 3-4 months
- 4-5 months
- 5-6 months

FIGURE **3-2**
**SOURCE LOCATION OF WATER
IN TUNNELS, 3-6 MONTHS**
PNC/TASK 5 REPORT/JAPAN



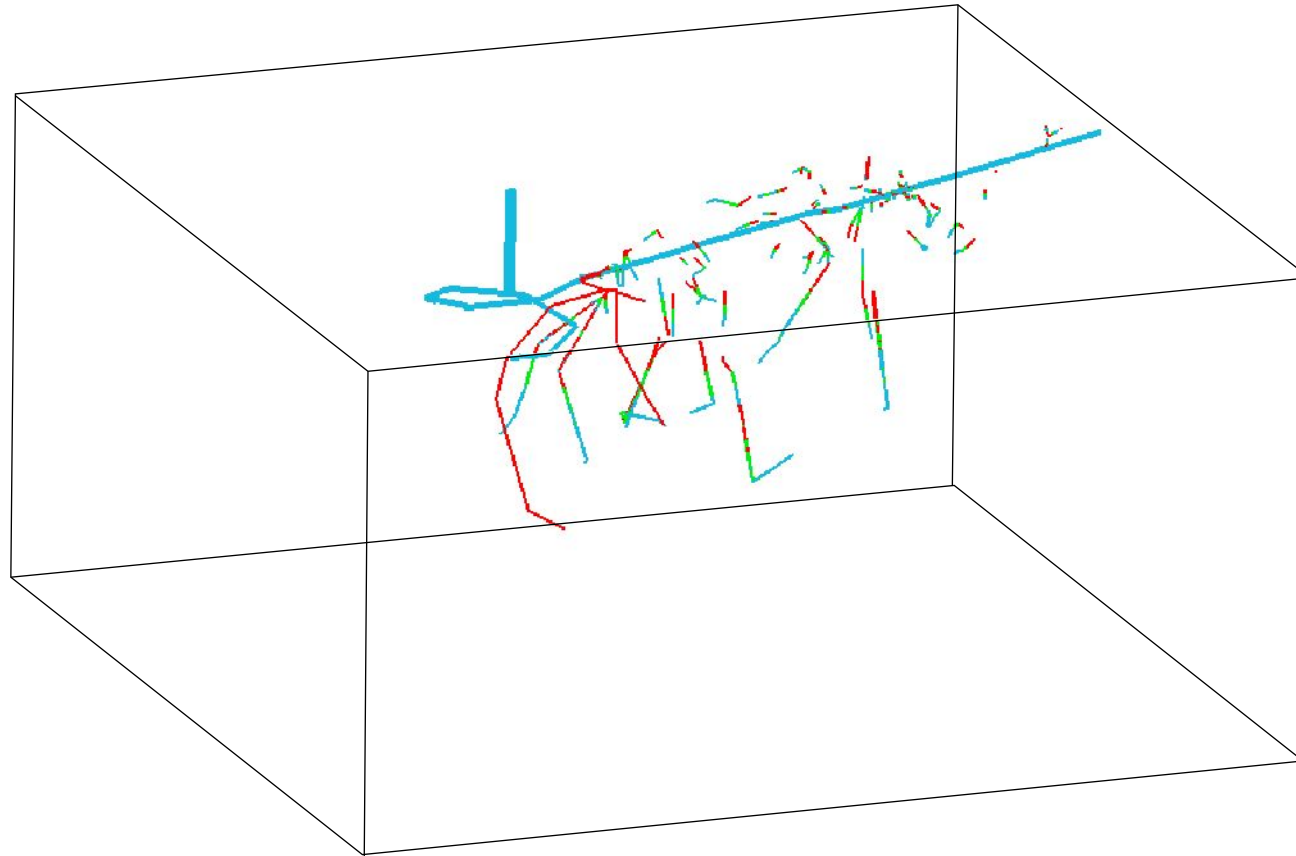
- 6-7 months
- 7-8 months
- 8-9 months

FIGURE 3-3
**SOURCE LOCATION OF WATER
IN TUNNELS, 6-9 MONTHS**
PNC/TASK 5 REPORT/JAPAN



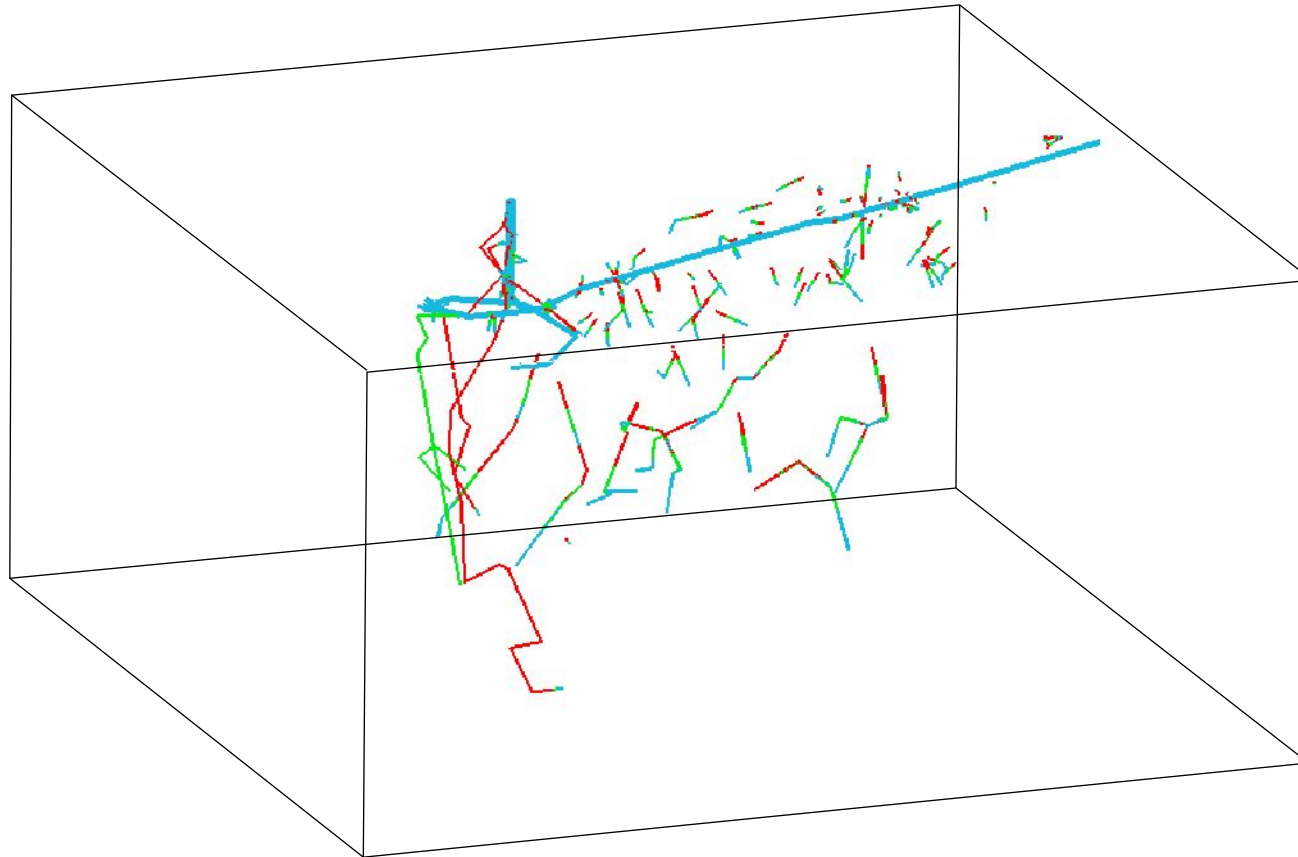
- 9-10 months
- 10-11 months
- 11-12 months

FIGURE **3-4**
**SOURCE LOCATION OF WATER
IN TUNNELS, 9-12 MONTHS**
PNC/TASK 5 REPORT/JAPAN



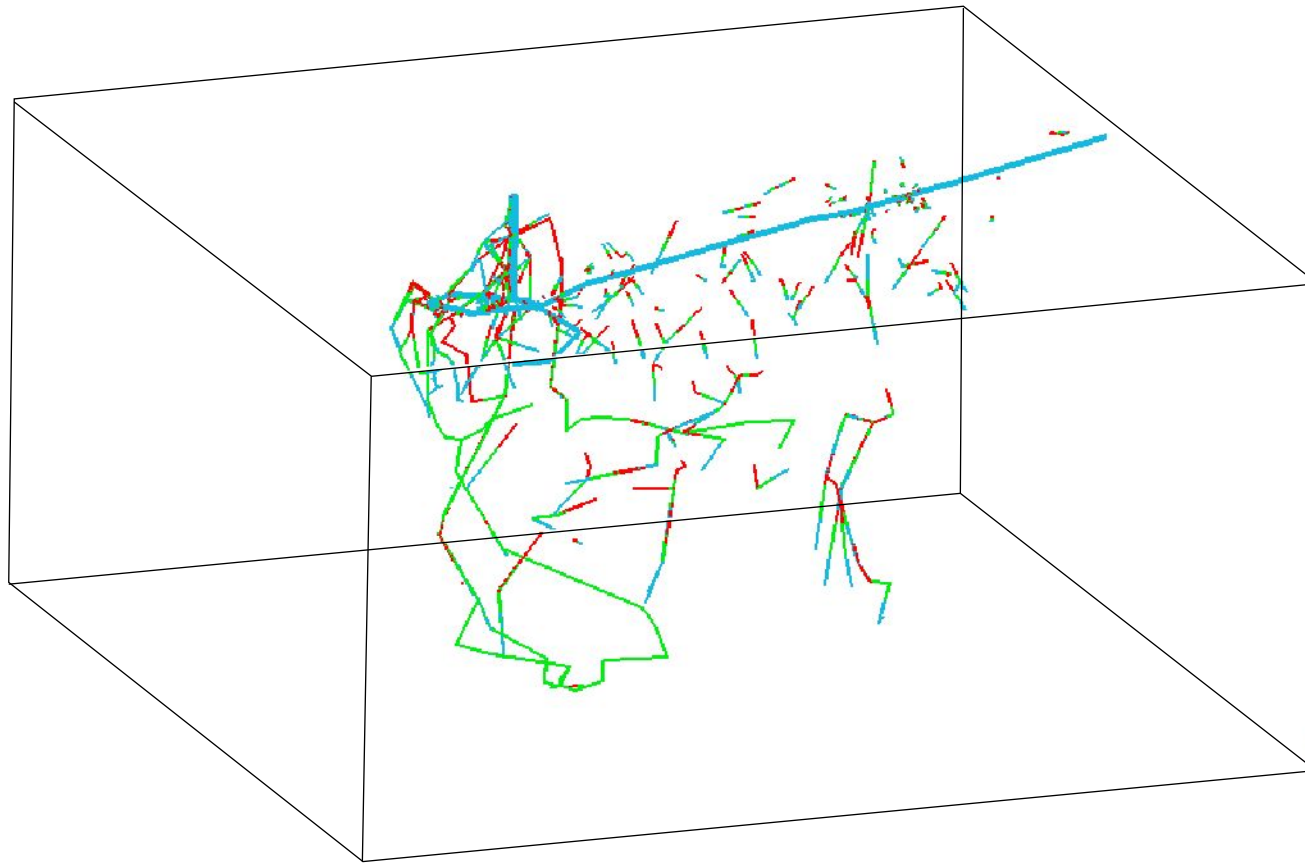
- 12-13 months
- 13-14 months
- 14-15 months

FIGURE **3-5**
**SOURCE LOCATION OF WATER
IN TUNNELS, 12-15 MONTHS**
PNC/TASK 5 REPORT/JAPAN



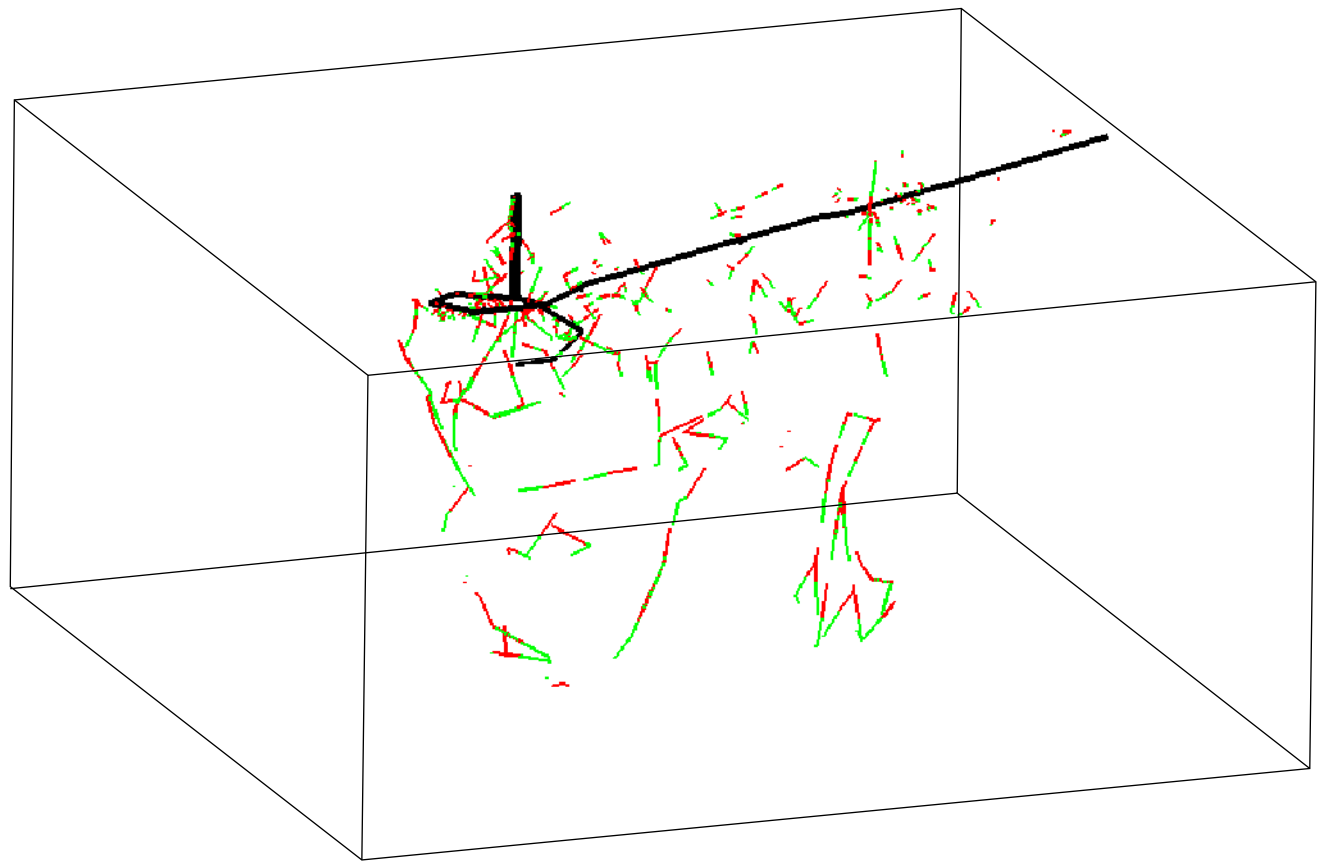
- █ 15-16 months
- █ 16-17 months
- █ 17-18 months

FIGURE **3-6**
**SOURCE LOCATION OF WATER
IN TUNNELS, 15-18 MONTHS**
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- 18-19 months
- 19-20 months
- 20-21 months

FIGURE **3-7**
**SOURCE LOCATION OF WATER
IN TUNNELS, 18-20 MONTHS**
PNC/TASK 5 REPORT/JAPAN



- 21-22 months
- 22-23 months

FIGURE **3-8**
**SOURCE LOCATION OF WATER
IN TUNNELS, 21-23 MONTHS**
PNC/TASK 5 REPORT/JAPAN

Fracture NE2a-1 (Weir 1745 m)

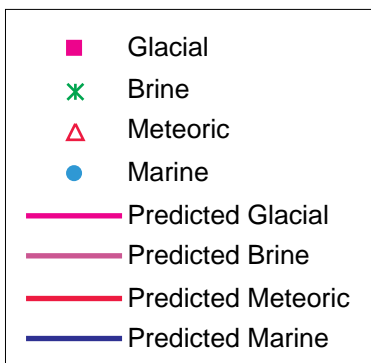
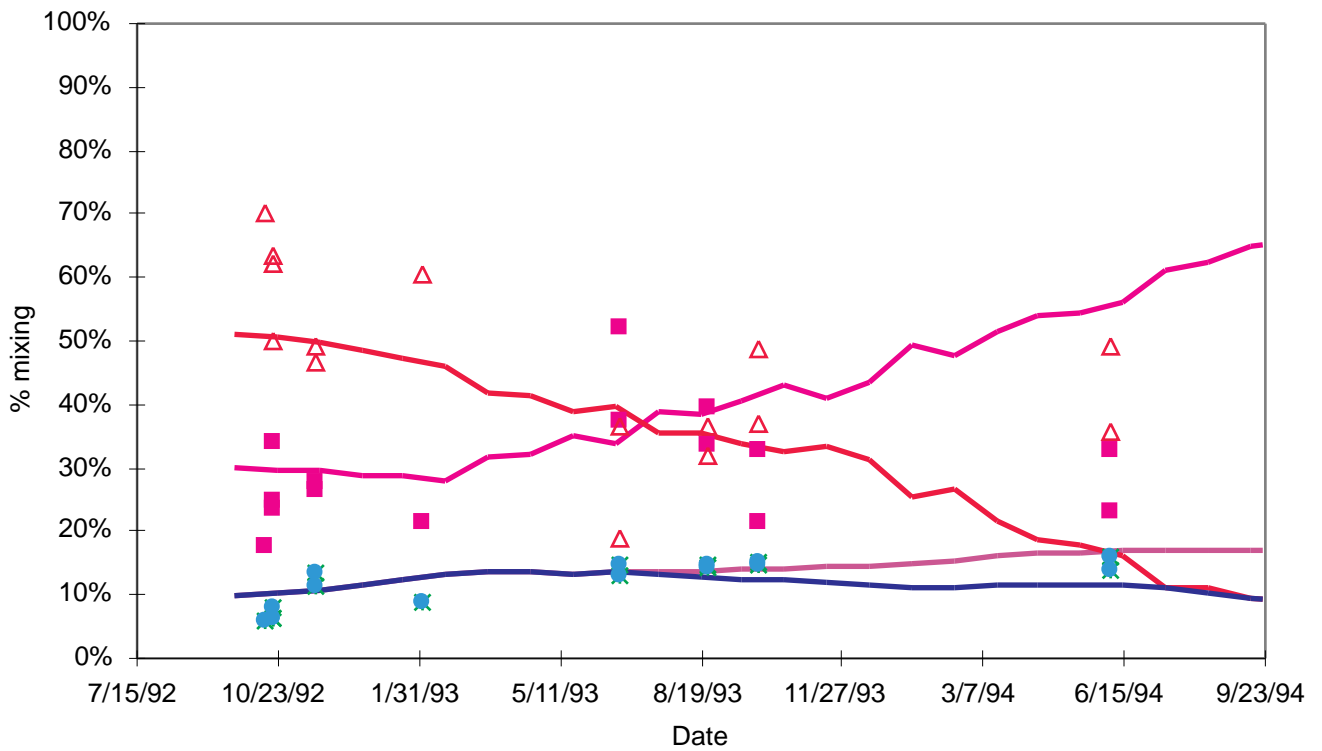


FIGURE 3-9
**END MEMBER BREAKTHROUGH,
 NE2a-1 CONTROL POINT**
 PNC/TASK 5 REPORT/JAPAN

NE-2a-2 (Weir 1883 m)

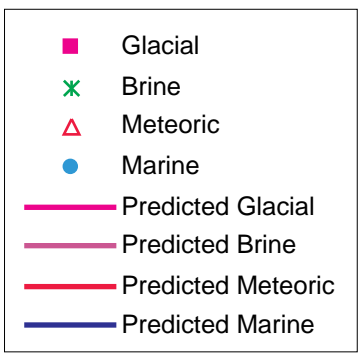
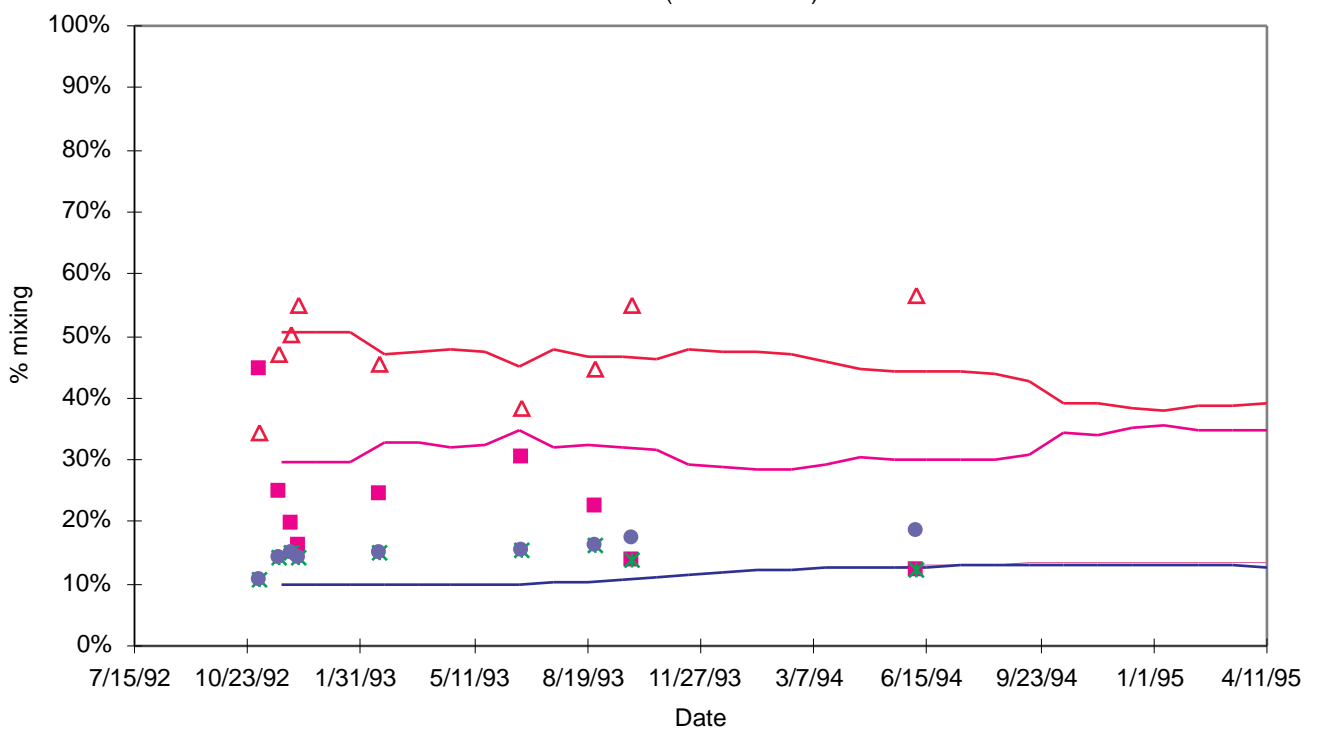


FIGURE 3-10
END MEMBER BREAKTHROUGH,
NE2a-2 CONTROL POINT
PNC/TASK 5 REPORT/JAPAN

NNW-4 H2O-1 (Weir 2178)

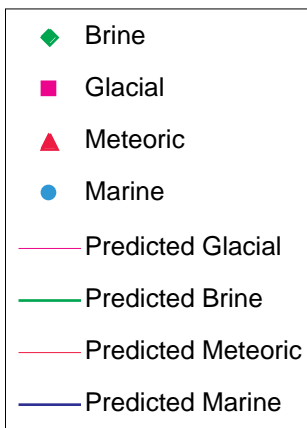
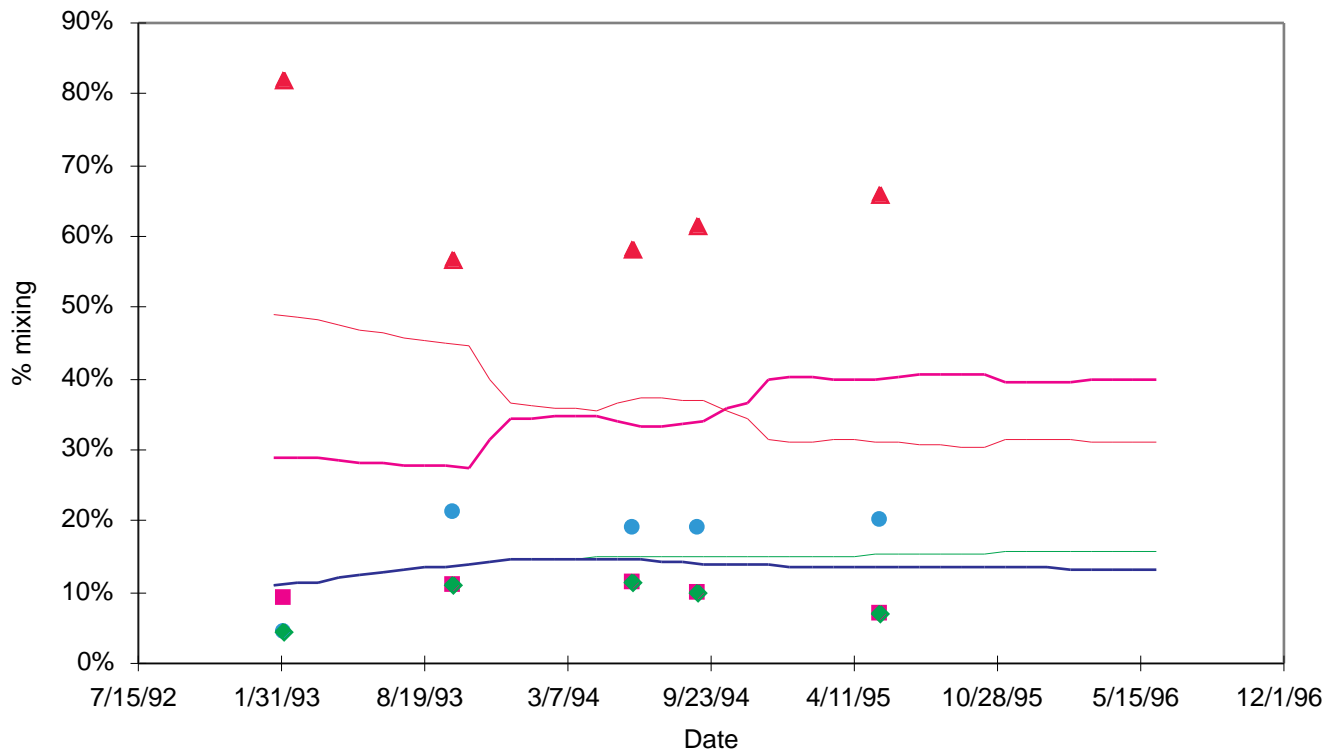


FIGURE **3-11**
END MEMBER BREAKTHROUGH,
NNW4, H2O-1 CONTROL POINT
 PNC/TASK 5 REPORT/JAPAN

NE2a-3 (Weir 2600 m)

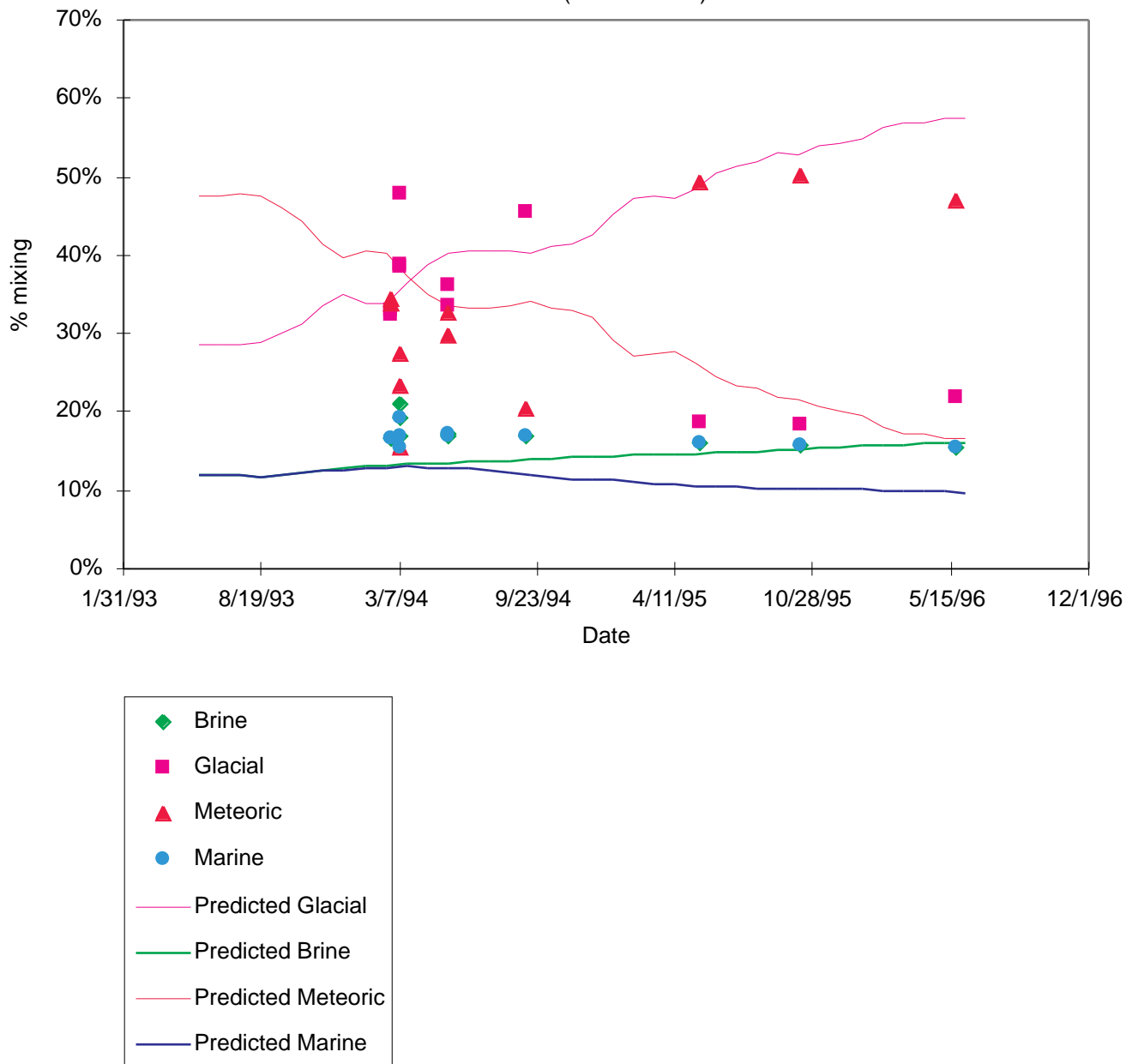


FIGURE 3-12
**END MEMBER BREAKTHROUGH,
 NE2a-3 CONTROL POINT**
 PNC/TASK 5 REPORT/JAPAN

4. CONCLUSIONS

The work described above successfully demonstrated that it is possible to apply PAWorks pathways analysis in the DFN model of Äspö to assess the source locations of the groundwater flow into the tunnels over time.

The results also indicate preferential upward flow from beneath the tunnels, which appears consistent with observed chloride response. However, this may be due to the assumed boundary conditions, and additional modeling is required to confirm this result.

Overall, the results of the preliminary Task 5 modeling indicate that PAWorks is a useful tool for deriving source locations of groundwater flow into the Äspö tunnels.

5. REFERENCES

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