

4/12

KELLEY ET AL

DOUBLE-POROSITY TRACER-TEST ANALYSIS FOR INTERPRETATION OF THE FRACTURE CHARACTERISTICS OF A DOLOMITE FORMATION

V.A. Kelley¹, J.F. Pickens¹, M. Reeves¹, and R.L. Beauheim²

¹INTERA Technologies, Inc.
6850 Austin Center Boulevard, Suite 300
Austin, Texas 78731

²Sandia National Laboratories
Albuquerque, New Mexico 87185

Abstract

Hydraulic and tracer testing studies have been performed as part of the regional hydrologic characterization of the Waste Isolation Pilot Plant (WIPP) site in southeastern New Mexico. The interpretation of hydraulic tests and tracer tests from a number of locations has indicated the importance of the double-porosity concept in the interpretation of both the hydraulic and solute-transport characteristics of the fractured dolomite under study. While identification of fracture flow and estimation of formation transmissivity can be obtained from hydraulic-test interpretation methods, tracer tests are necessary to provide realistic estimates of parameters such as fracture porosity and representative matrix unit size. Without estimates of these parameters, predictions of contaminant transport in fractured rock systems are very uncertain.

A convergent-flow tracer test conducted in the Culebra Dolomite Member of the Rustler Formation at the WIPP site was analyzed using a double-porosity flow and transport model. The tracer test set-up consisted of one pumping well and two tracer-addition wells arranged in an approximate equilateral triangle with 100-ft (30-m) sides. The transport of conservative tracers from each of the tracer-addition wells was simulated using the double-porosity flow and transport model SWIFT II. The simulation model accounts for advective-dispersive transport in the fractures and diffusive transport in the matrix. Calibration of the tracer-breakthrough curves included conducting a sensitivity analysis on the important parameters: diffusion coefficient, tortuosity, matrix porosity, fracture porosity, effective matrix-block size, pumping rate.

102-8
WM-11
NH03

initial tracer input distribution, and distance between pumping and tracer-addition wells. Calibration of the tracer-breakthrough curves resulted in longitudinal dispersivities from 5 to 10% of the flow path length (well-separation distance), a fracture porosity of 0.002, and effective matrix-block sizes of 0.8 ft (0.25 m) to 3.9 ft (1.2 m). Even though these estimates of fracture porosity and effective matrix-block size are specific to the location of the tracer test, they provide an initial estimate on which to base predictions of the regional transport of solutes in the Culebra dolomite.

1.0 Introduction

Hydraulic and tracer-testing activities have been performed as part of the regional hydraulic characterization studies for the Waste Isolation Pilot Plant (WIPP) site in southeastern New Mexico. The WIPP site is located approximately 26 miles (42 km) east of Carlsbad, New Mexico (Figure 1). The site characterization studies are being coordinated by Sandia National Laboratories on behalf of the Department of Energy and involve the evaluation of the suitability of bedded salt of the Salado Formation for isolation of defense transuranic wastes.

The Culebra dolomite is the most transmissive rock unit above the waste-emplacement horizon (Mercer, 1983) and for this reason it has been the main focus of site-characterization studies at the WIPP site. The Culebra dolomite in portions of the WIPP-site area is considered to be a fractured rock possessing both primary and secondary porosity (Rehfeldt, 1984; Chaturvedi and Rehfeldt, 1984; Beauheim, 1987 and Kelley and Pickens, 1986). The hydraulic and tracer-testing methods and interpretation approaches have allowed quantification of fracture flow and transport properties.

The H-3 hydropad is a well nest composed of three wells, and is located in the south-central part of the WIPP site approximately 3900 feet (1190 m) south of the repository waste-handling shaft (Figure 1). Transport-parameter characterization of the Culebra at the H-3 hydropad is considered important because (1) the hydropad is located on a potential flow path from a repository breach under natural ground-water flow conditions, and (2) the hydropad is a potential site for the implementation of a sorbing-tracer test (Pearson et al., 1987). Both hydraulic and tracer tests have been interpreted using double-porosity models at the H-3 hydropad (Beauheim, 1987; Kelley and Pickens, 1986). The double-porosity interpretation for a conservative-tracer test is presented here with the interpretation reviewed for its consistency with the physical system. The suitability of hydraulic and tracer tests to determine appropriate double-porosity flow and transport parameters for the Culebra dolomite at the H-3 hydropad is also discussed.

2.0 Site Characterization

2.1 Hydrogeology of the Culebra Dolomite Member

The sediments underlying the WIPP site range in age from Ordovician to Recent. The sediments that are of most interest for characterizing the performance of the WIPP repository are of Permian age and were laid down

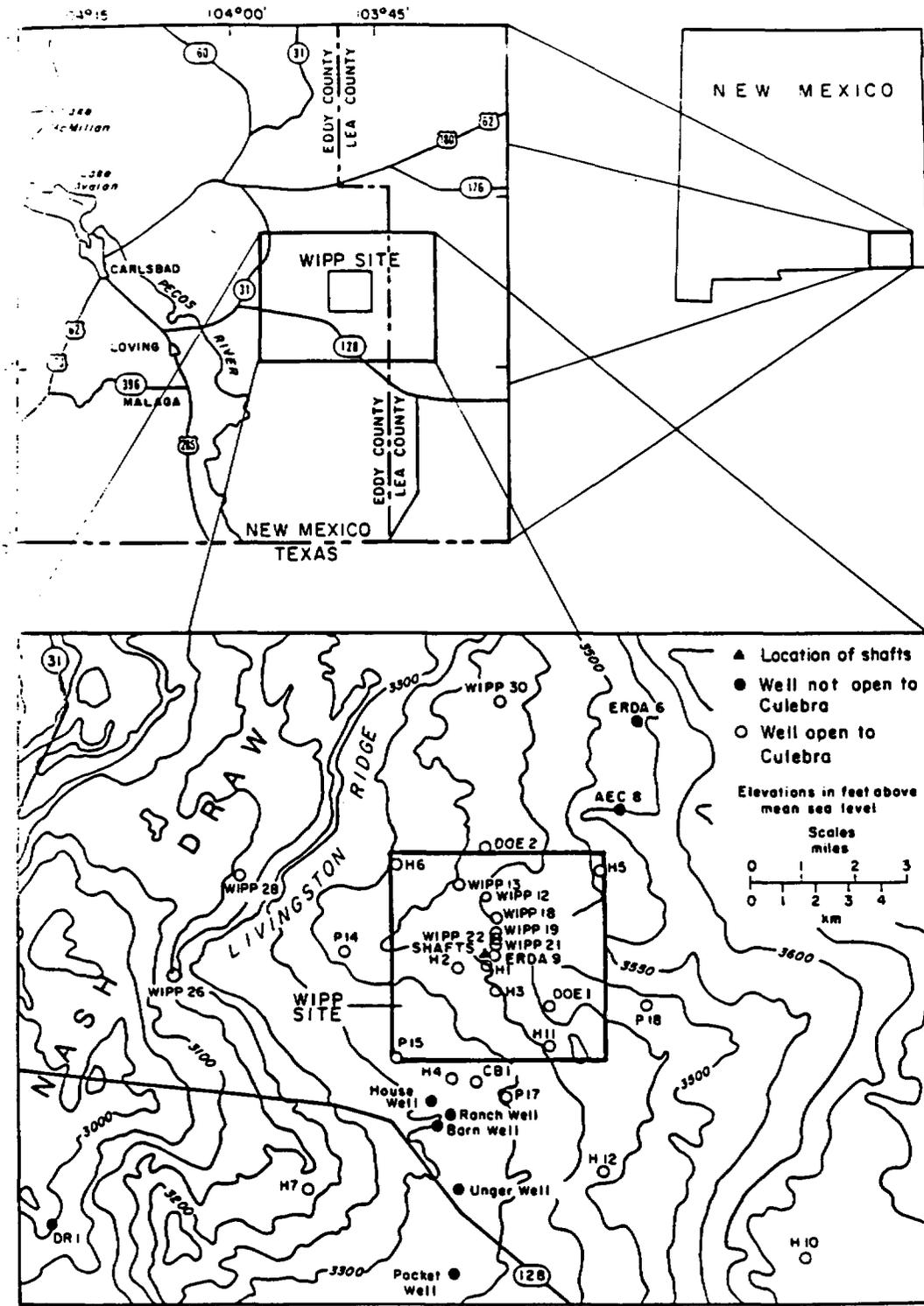


Figure 1 Site Location for the Waste Isolation Pilot Plant Showing the Hydropad Observation-Well Network for Regional Hydrogeologic Characterization

in a deep-water embayment of the Permian depocenter known as the Delaware Basin. The Salado Formation is a thick-bedded salt section within which the waste repository will be located. Immediately above the Salado Formation is the Rustler Formation, which is divided into five members based on lithology (Vine, 1963). Of these five, the Culebra Dolomite Member is considered to be the most transmissive unit (Mercer, 1983).

The Culebra dolomite at the H-3 hydropad is 23 ft (7 m) thick and is locally fractured. Interpretations of a 14-day pumping test in 1984 and a 62-day pumping test in 1985 have yielded transmissivities of 3.0 and 1.8 ft²/day (3.2×10^{-6} and 1.9×10^{-6} m²/s), respectively (Beauheim, 1987). Beauheim (1987) also concluded that the Culebra responded hydraulically as a double-porosity medium at the H-3 hydropad and that the pumping wells in both tests were intersected by fractures which substantially increased the production surface available to each of the wells. The hydraulic gradient under undisturbed conditions (before shaft construction) at the H-3 hydropad is estimated to be 4×10^{-3} to the south-southeast (Haug et al., 1987). Ground water from the Culebra at the H-3 hydropad has a density equal to 64.8 lbm/ft³ (1038 kg/m³) (INTERA, 1986). A modeling study providing a regional evaluation of ground water flow in the Culebra at the WIPP site is presented by Haug (1987).

2.2 Characterization of the Fracture Properties of the Culebra

Little quantitative information is available concerning the geometry of fractures in the Culebra, although several publications discuss their presence. From a review of some articles which do offer a degree of quantitative information (Ferrall and Gibbons, 1980; Black et al., 1983; Holt and Powers, 1984; Rehfeldt, 1984; and Core Laboratories, Inc., 1986a), the following general conclusions were made: (1) both high-angle and horizontal fractures are present; (2) fracture apertures up to 0.3 cm were observed within the original ventilation shaft at the WIPP site (now the waste-handling shaft); (3) fracture lengths from centimeters to a maximum of 2.1 m were observed in the original ventilation shaft; (4) when filled, fractures are most commonly filled with gypsum, yet in some cases they are lined with oxides, pyrite, or bitumen; and (5) fracture faces examined in core analysis possess surface textures and mineralization indicative of fluid movement.

The range of fracture spacings to be utilized in modeling studies should be derived from information that is as site specific as possible. The best source of site-specific information is the description of the core obtained from two of the three Culebra wells at the H-3 hydropad. Core recovery at the H-3 hydropad was very poor (Figure 2). Therefore, one must be discerning drawing conclusions from such a limited data base. Approximately 10 percent of the Culebra interval was recovered in the coring of the borehole designated H-3b2 and approximately 40 percent of the Culebra interval was recovered in the coring of the borehole designated H-3b3. At the H-3 hydropad, greater than 50 percent of the fractures are observed to be open in the recovered core. Both horizontal and vertical fractures are present. There are no recovered pieces of core longer than 1 ft (0.3 m) in length and the core appears very porous. Because of potential core destruction during coring, estimation of an upper matrix-block size is not reasonable, however it is felt that

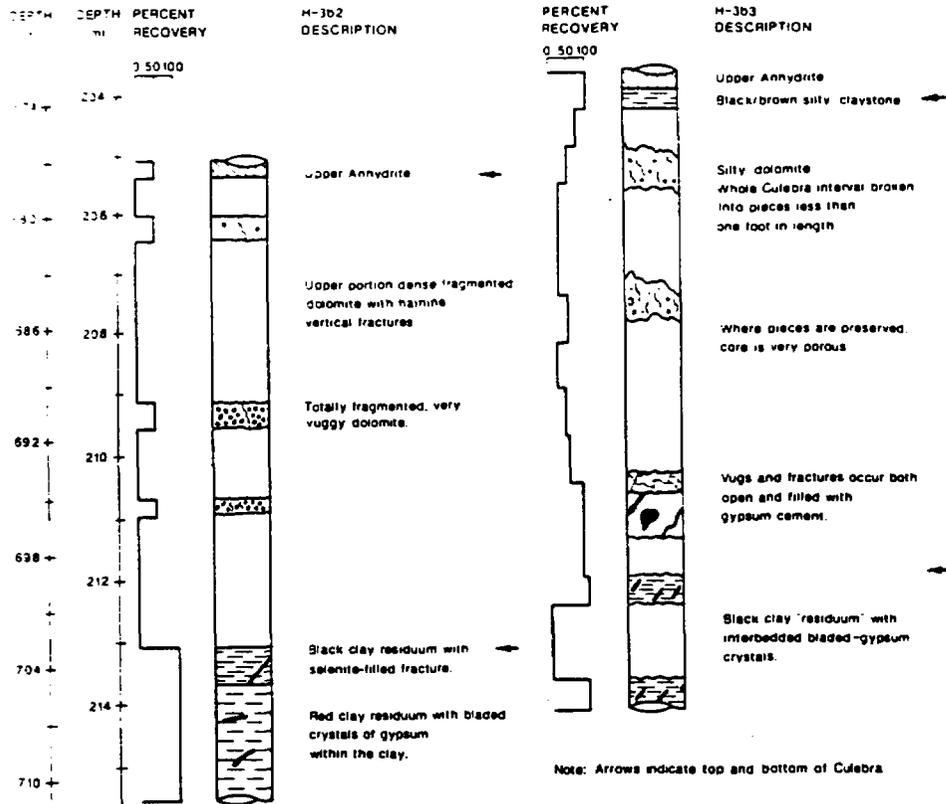


Figure 2 Results of Core Examination of Culebra Dolomite from Boreholes H-3b2 and H-3b3

the minimum matrix-block size can be estimated for the portions of the Culebra with recovered core. Through review of core and core photographs, 0.5 ft (0.15 m) is considered a reasonable lower limit for matrix-block size.

3.0 H-3 Hydropad Tracer Test

3.1 Well Configurations and Downhole-Equipment Assemblies

A convergent-flow tracer test was conducted at the H-3 hydropad from May 16 to June 13, 1984 by Hydro Geo Chem, Inc., under contract to Sandia National Laboratories. The H-3 hydropad consists of three wells, H-3b1, H-3b2, and H-3b3, arranged in an approximate equilateral triangle with 100-ft (30.5-m) sides. A borehole deviation survey was performed at the H-3 hydropad and the distances between boreholes at the Culebra depth are: H-3b1 to H-3b2 equal to 91.3 ft (27.8 m); H-3b2 to H-3b3 equal to 87.9 ft (26.8 m); and H-3b3 to H-3b1 equal to 100.6 ft (30.7 m) (Saulnier et al., 1987).

Figure 3 shows the downhole configuration of the three H-3 hydropad wells during the tracer-testing sequence. In the pumping well (H-3b3), a submersible pump was installed below a Baski air-inflatable

sliding-end packer, with the discharge line extending through the packer and then to ground surface. A packer and feed-through plug were also used in the H-3b2 tracer-addition well during the tracer test. The packer system also served to minimize the system volume during tracer addition by isolating the wellbore fluid in the annular space above the test interval from the downhole system volume (see Figure 3). Fluid pressure was measured in each borehole with Druck PDCR-10 pressure transducers.

Tracers were injected into wells H-3b1 and H-3b2 from the surface through 1/2-inch (1.3-cm) polyethylene tubing. For H-3b1, the polyethylene tube was lowered inside the 2-3/8-inch tubing string to a depth of 525 ft (160 m) below top of casing, where it encountered an apparent obstruction preventing positioning of the tube to a lower depth. In well H-3b2, the 1/2-inch polyethylene injection tube was fed through the packer feed-through plug to allow injection to the zone below the packer.

3.2 Tracers

The tracers used in the H-3 hydropad tracer tests, pentafluorobenzoate (PFB) and meta-trifluoromethylbenzoate (m-TFMB), are anhydrous acids derived from benzoic acid. PFB has been tested extensively, both in the field and in the laboratory, and has not shown evidence of sorption or

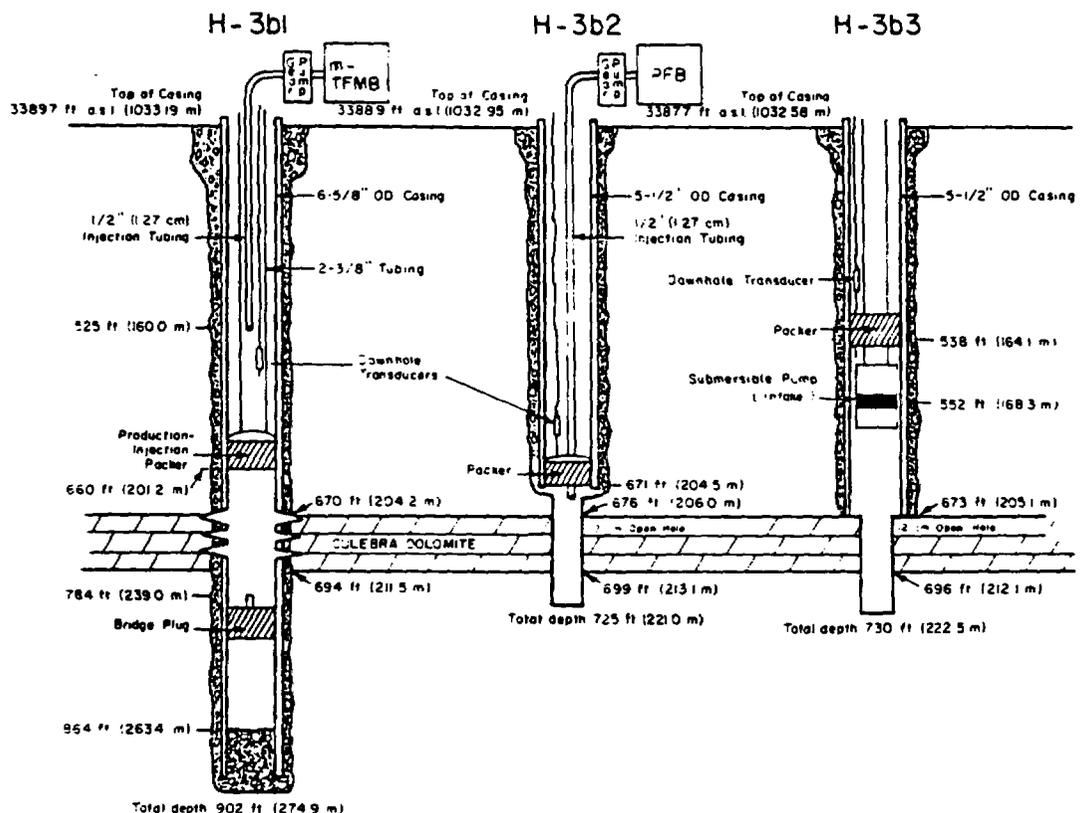


Figure 3 Schematic Representation of the Downhole Configuration at the H-3 Hydropad During the Tracer Test

degradation (Stetzenbach, personal communication). m-TFMB has also been tested extensively and shows no signs of sorption. Experiments carried out at the University of Arizona have shown it to be resistant to degradation for at least six months (Stetzenbach, personal communication). Hydro Geo Chem (in preparation) used five fluorinated benzoic acid tracers in tracer tests performed at another location at the TRPP site and concluded that only m-TFMB and PFB showed no signs of degradation. These two tracers have the additional strong points of being (1) exotic to the Culebra ground water at the H-3 hydropad, and (2) detectable at very low concentration levels through proven analytical techniques (Stetzenbach et al., 1982).

3.3 Tracer-Test History

The H-3 hydropad tracer test was a convergent-flow tracer test in which well H-3b3 was pumped at a nominally constant rate of 3 gpm (0.19 l/s), while 2.2 lb (1 kg) of tracers m-TFMB and PFB were injected with 100 gal (379 l) and 60 gal (227 l) of formation fluid, respectively, over a 1.6-hour period into wells H-3b1 and H-3b2, respectively. The breakthrough curves obtained for the m-TFMB and PFB tracers from water samples from the pumping well H-3b3 are shown in Figure 4, and the arrival times, first-measured and peak concentrations, and percent tracer recovery at the pumping well are summarized in Table 1.

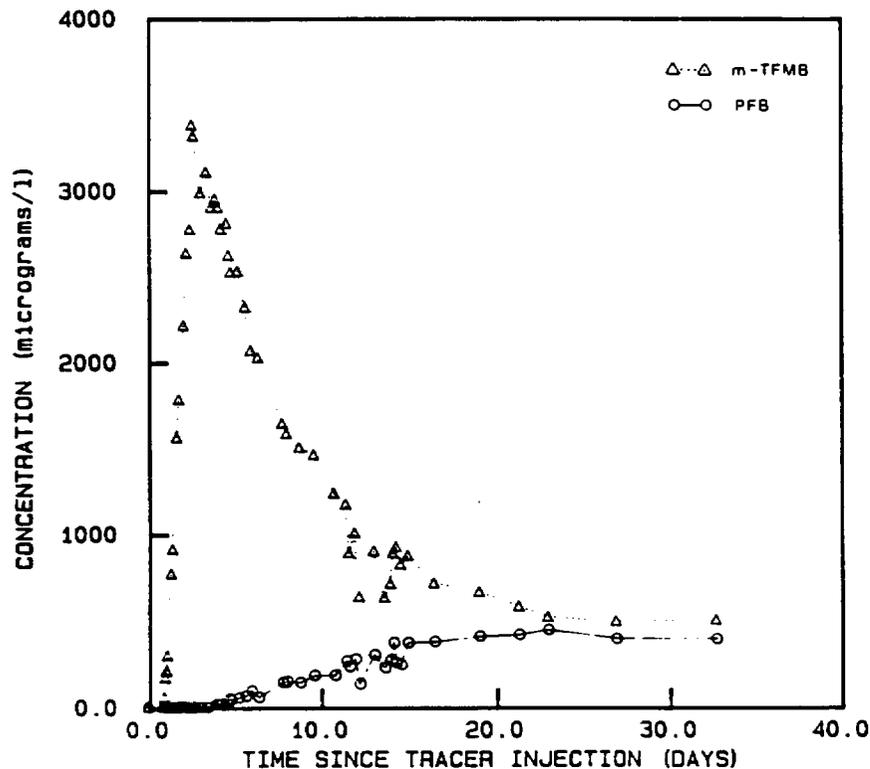


Figure 4 Tracer Concentrations at the Pumping Well for PFB and m-TFMB Expressed as Micrograms per Liter

First detection of m-TFMB (reported concentration of 56 µg/l) at the pumping well was obtained from water samples taken 22.1 hours (0.92 days) after tracer injection at well H-3b1. The maximum observed concentration (3379 µg/l) was recorded 62.08 hours (2.59 days) after tracer injection. By integrating for the mass below the m-TFMB breakthrough curve over the duration of the test, it is estimated that approximately 53 percent of the injected tracer mass was recovered at the pumping well. First detection of PFB (reported as trace concentration) at the pumping well was obtained from water samples taken 90.25 hours (3.76 days) after tracer injection at well H-3b2. The maximum observed concentration (444 µg/l) was recorded 553 hours (23.04 days) after injection (Figure 4). By integrating for the mass below the PFB breakthrough curve over the duration of the test, recovery of approximately 15 percent of the injected tracer mass is estimated. The PFB breakthrough curve exhibits a peak concentration about a factor of eight lower than the m-TFMB breakthrough curve and a time to reach the peak concentration delayed by a factor of nine when compared to the m-TFMB breakthrough curve.

3.4 Interpretation Approach

The objectives of the interpretation of the H-3 tracer test were to develop a consistent conceptualization of the governing physical solute-transport processes operating in the Culebra at the H-3 hydropad and to develop quantitative estimates of the respective transport parameters.

From a review of the information base for the H-3 hydropad, it was concluded that a double-porosity interpretation approach was the most appropriate. This information base included: (1) identification of open fractures in core samples; (2) very rapid transport rate between the

Table 1 Summary of Tracer Arrival Times and Mass Recoveries at the Pumping Well H-3b3

Parameter	Tracer	
	m-TFMB	PFB
Flow Path	H-3b1 to H-3b3	H-3b2 to H-3b3
First reported concentration (µg/l)	56	20
Time of first detection (days)	0.92	3.76
Time of arrival of peak concentration (days)	2.59	23.04
Peak concentration (µg/l)	3379	444
(M/M)	2.9×10^{-6}	3.5×10^{-7}
Tracer mass recovered during the test (%)	53	15

tracer-addition wells and the pumping well; and (3) the identification of fracture flow and a double-porosity pressure response from the analysis of the pumping test at the H-3 hydropad (Beauheim, 1987).

Because of the relatively high matrix porosity of the Culebra, solute transport between the fractures and the matrix by diffusion is expected to be a significant process. Therefore, a discrete fracture model with transport in the fractures only is not considered an appropriate conceptualization for analyzing the H-3 tracer test. The double-porosity approach is considered appropriate and is described below.

The concept of a double-porosity medium was first proposed by Earenblatt et al. (1960) to model flow in fractured rock. Inherent to the concept of a double-porosity medium is the idea that the medium consists of two separate, interacting and overlapping continua. Using the Streltsova-Adams (1978) classification for dual-porosity reservoirs, the Culebra at the H-3 hydropad is a class-one dual-porosity reservoir which is termed a fractured medium. In a fractured medium, the primary medium (the matrix) has the greater porosity and effectively represents the bulk of the "storage" capacity of the unit, and the secondary medium (the fractures) has "transport" properties generally as a result of secondary processes (i.e., post-depositional). Also inherent in double-porosity theory is the concept that any representative finite volume of the collective media contains both primary and secondary media.

In a double-porosity medium, various assumptions are necessary to allow the system to be represented mathematically. One very important assumption is that the system can be characterized as fractures and matrix units with a relatively simple interaction between them. The Culebra is assumed to have three orthogonal fracture sets. This fracture/matrix system is modeled as spheres. Spheres are advantageous because the cubic grid geometry is awkward for modeling internal diffusion. This problem is solved by approximating the cube matrix units by spheres having the same surface-to-volume ratio as a cubic block (Neretnieks, 1980; Rasmuson and Neretnieks, 1981; Rasmuson et al., 1982). Neretnieks (1972) found that this approximation yields the equivalent uptake as cubes for short times and only varies slightly for larger times. While these mathematical idealizations cannot be expected to represent natural geologic systems exactly, they do allow the solution for double-porosity transport at the field scale to be a tenable problem. Conceptually, one should consider these ideal representations as approximations of the natural system, where one is attempting to attain quantitative consistency between the fracture fluid volume and the surface area available for diffusion.

Further assumptions were made regarding the conceptual basis for this analysis. The flow field in the study area was assumed to be radial around the pumped well and at steady-state conditions during the tracer test. Since the hydraulic conductivity of the matrix is low and the flow regime is approximately at steady state, advective transfer from the fractures to the matrix and advective transport in the matrix were assumed to be negligible. Therefore, the transport of the tracer from the fractures to the matrix and within the matrix was assumed to occur by diffusion only. The double-porosity medium was assumed to be homogeneous and isotropic.

The SWIFT II model was selected for simulation of the tracer tests performed at the H-3 hydropad. SWIFT II is a fully-transient, three-dimensional, finite-difference code capable of solving the coupled equations for flow and transport in a double-porosity medium. A comprehensive description of the theory and implementation of the SWIFT II model is presented in Reeves et al. (1986).

The transport equations were solved in a radial coordinate system. A Cartesian coordinate system would be impractical because of the very large number of grid blocks and time steps that would be required to prevent numerical problems. Additional reasons for choosing the radial approach to simulate the H-3 tracer test are: (1) it offers advantages in meeting the numerical criteria of the model, and (2) the field data base on heterogeneity is not sufficient to warrant utilizing the Cartesian approach, which is much more difficult to implement.

A schematic representation of the global discretization in both plan view and cross section is shown in Figure 5 for the pumping well and a typical tracer-addition well. The pumping well resides at the center of the radial system and is given a constant discharge rate consistent with that measured during the tracer test. Both upper and lower boundaries of

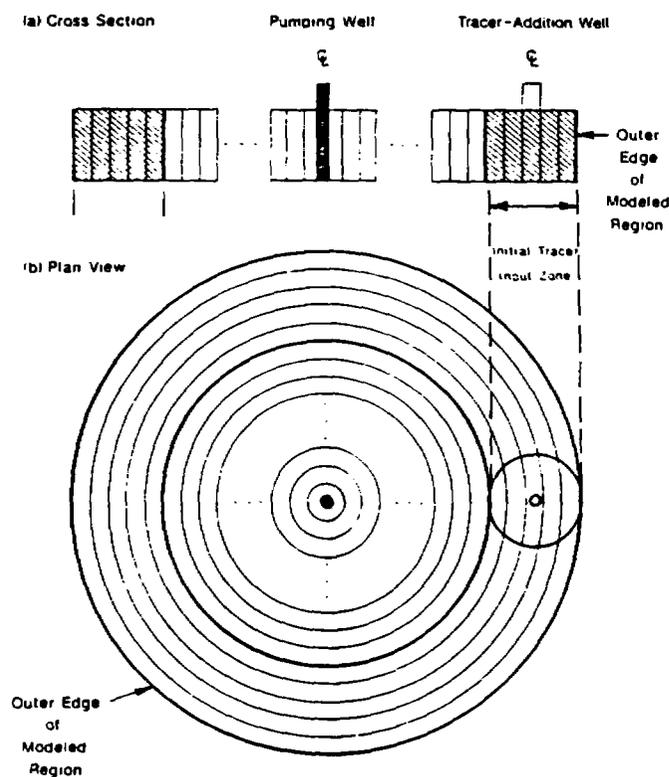


Figure 5 Schematic Representation of the Modeled Region, (A) Cross Section, (B) Plan View

the system are considered to be no-flow boundaries. At the outer edge of the radial system, a Dirichlet pressure boundary condition is prescribed. Using the radial simulation approach, the initial tracer distribution surrounding the tracer-addition well is approximated as being distributed in a concentric ring surrounding the pumping well. The actual radial tracer-input zone at the end of the short-duration tracer-addition phase and the approximated zone for modeling purposes are shown schematically in Figure 5. Further details on the calculation procedures for estimating the mass of tracer introduced into each of the global grid blocks at the input zone are outlined in Kelley and Pickens (1986).

The radial discretization implemented for the global system assumes that the geologic system is both homogeneous and isotropic. As a result, flow paths for tracers m-TFMB and PFB were analyzed separately. Results from anisotropy determinations from pumping tests performed at the H-4, H-5, and H-6 hydropads at the WIPP site (Gonzalez, 1983) have yielded anisotropy ratios of 2.7:1, 2.4:1, and 2.1:1. This degree of anisotropy is weak in magnitude and cannot clearly be differentiated from the effects of aquifer heterogeneity. Although it is felt that hydropad-scale heterogeneities are present at the H-3 hydropad, the quantification of the spatial variability of the medium properties is not possible from the existing information base.

3.5 Model Input Parameters

As discussed earlier, the Culebra dolomite at the H-3 hydropad is conceptualized as a double-porosity system for solute-transport modeling purposes. Parameters characterizing the Culebra, tracers, tracer-test operating conditions, fractures, and matrix were utilized in fitting the m-TFMB and PFB breakthrough curves determined from water samples taken from the pumping well. The following is a discussion of the estimation of values for each of these parameters.

Tracer Free-Water Diffusion Coefficient

Free-water diffusion coefficients for m-TFMB and PFB have been reported by Walter (1982). He calculated the free-water diffusion coefficients using the Nernst expression and data from laboratory experiments conducted to determine the limiting ionic conductances of the tracer species. The calculated diffusion coefficients for m-TFMB and PFB were $6.9 \times 10^{-4} \text{ ft}^2/\text{d}$ ($7.4 \times 10^{-6} \text{ cm}^2/\text{s}$) and $6.7 \times 10^{-4} \text{ ft}^2/\text{d}$ ($7.2 \times 10^{-6} \text{ cm}^2/\text{s}$), respectively (Walter, 1982).

Tortuosity

The solute diffusion coefficient in the porous matrix is defined as follows for use in the SWIFT II code:

$$D^* = \phi_m \tau D_o \quad (1)$$

where D^* is equal to the solute molecular diffusivity in the porous matrix; ϕ_m is equal to the matrix porosity; τ is equal to the tortuosity; and D_o is equal to the free-water diffusion coefficient. In studying solute transport by diffusion, tortuosity is a parameter whose

magnitude ($0 < \tau < 1$) is a measure of the tortuous nature of the pores through which the solute is diffusing. As the resistance to diffusional transport for a conservative species increases, the magnitude of tortuosity decreases. Bear (1972) has presented a review of tortuosity values in the range of 0.3 to 0.7. Bear states that tortuosity is correctly defined as:

$$\tau = (L/L_e)^2 \quad (2)$$

where L is equal to the straight-line distance; and L_e is equal to the mean length of the diffusional path in a porous matrix.

Although not stated, Bear's review appears to have been for studies utilizing unconsolidated media. Reported tortuosity values for consolidated materials like dolomite are rare. Tortuosity values of 0.02 to 0.17 were calculated from the diffusion coefficients of Cl^- in chalk samples by Barker and Foster (1981). From diffusion experiments on crystalline rock samples, Katsube et al. (1986) calculated tortuosity values of 0.02 to 0.19. It is expected that the tortuosity will vary spatially within the Culebra. For simulation purposes in interpreting the tracer test at the H-3 hydropad, tortuosity values of 0.15 and 0.45 were chosen.

Longitudinal Dispersivity

In fitting tracer-breakthrough curves for transport in a single-porosity medium, longitudinal dispersivity is often the key parameter utilized in the calibration (i.e., fitting breakthrough-curve shape and peak concentration). In a double-porosity system, the transport of solutes between the fractures and matrix by diffusion can have a very large effect on the breakthrough curve, thus causing the interpretation of the best-fit longitudinal dispersivity to be difficult. A review of the literature on the magnitude of longitudinal dispersivity for various tracer-test scales and contamination-plume sizes (e.g., Lallemand-Barres and Peaudecerf, 1978; Pickens and Grisak, 1981) suggests that longitudinal dispersivity can be expressed as a function of the mean travel distance of the tracers or contaminants. In many situations, the longitudinal dispersivity is from 5 to 10 percent of the travel-path length. Since the well spacings at the H-3 hydropad were approximately 100 ft (30 m), longitudinal dispersivities of 4.9 ft (1.5 m) to 9.8 ft (3.0 m) were chosen for simulation of the breakthrough curves.

Fracture Porosity

From examination of the tracer-breakthrough curves, it was concluded that the rapid arrival of the m-TFMB tracer at the pumping well could have been dominated by transport in fractures along the H-3b1 to H-3b3 flow path. A first estimate for the fracture porosity was calculated from the relation

$$\phi_f = Q\bar{t} / \pi r^2 h \quad (3)$$

where ϕ_f is equal to the fracture porosity; Q is equal to the discharge rate at the pumping well; \bar{t} is equal to the time to reach the peak

concentration; r is equal to the distance between the tracer-addition and pumping wells; and h is equal to the aquifer thickness. This equation is based on the assumption that transport is occurring in the fractures only with no tracer losses to the matrix. Therefore, it will yield an overestimate for the fracture porosity.

Using equation 3, the calculated fracture porosity based on the m-TFMB breakthrough curve for the H-3b1 to H-3b3 flow path was approximately 2.0×10^{-3} . The PFB breakthrough curve for the H-3b2 to H-3b3 flow path exhibited a much later first detection of tracer and did not have a well-defined peak concentration. Therefore, only the fracture porosity determined from the m-TFMB breakthrough curve was utilized. Because of the large difference between the breakthrough curves for m-TFMB and PFB, it is recognized that the estimated fracture porosity is uncertain and its representativeness to both flow paths may be questionable.

Matrix Porosity

Porosity determinations conducted on six core samples from boreholes H-3b2 and H-3b3 ranged from 0.11 to 0.24 (Core Laboratories, 1986b) with an average value of approximately 0.2. A matrix porosity of 0.2 was chosen for simulating the tracer-breakthrough curves.

Matrix-Block Size

As discussed in Section 3.4, the conceptualization of the double-porosity system involves mathematically representing the natural system as a homogeneous, idealized configuration of fractures and matrix units. For modeling the tracer-breakthrough curves at the H-3 hydropad, the matrix units were assumed to be defined by three orthogonal fracture sets. Both horizontal and vertical (or near vertical) fracture sets have been observed in core samples, shaft excavations, and outcrop areas. Even though the natural system is heterogeneous, one must attempt to develop a reasonable approximation of the correct fracture fluid volume and the surface area available for diffusion from the fractures to the matrix.

A spherical representation of the matrix units was chosen for simulation purposes. Because the time scale of the tracer tests is not very long, with the depth of penetration of the tracer into the matrix units not large, the spheres are mathematically equivalent to the cube representation through a consistent correlation of fracture fluid volume and surface area available for diffusion. This assumption in the simulation approach is discussed further by Kelley and Pickens (1986).

The characteristic matrix-unit size (i.e., fracture spacing) is expected to vary considerably over the WIPP-site area and also vertically at any location as a result of the high degree of heterogeneity observed in the Culebra. Matrix-block sizes from 0.5 ft (0.15 m) to 3.3 ft (1.0 m) are considered a reasonable range based on examination of core samples. These matrix-block sizes were utilized as initial estimates for simulating the tracer-breakthrough curves using the SWIFT II model.

Pumping Rate

The discharge rate at the pumping well was relatively constant at 3 gpm (0.19 l/s) throughout the tracer test. This pumping rate was used to simulate the tracer-breakthrough curves.

Culebra Thickness

The definition of the bottom and top of the Culebra has been reviewed using available geophysical logs (Beauheim, personal communication). At H-3b1 the Culebra thickness is 24 ft (7.3 m), at H-3b2 it is 23 ft (7.0 m), and at H-3b3 it is 23 ft (7.0 m). A Culebra thickness of 23 ft (7.0 m), corresponding to the thickness estimate at the pumping well, was chosen for simulating the tracer-breakthrough curves.

Distance Between Tracer-Addition and Pumping Wells

Distances between the boreholes at the Culebra depth were calculated based on the surveys of the borehole locations at ground surface and borehole-deviation surveys (Saulnier et al., 1987). The distances between H-3b1 and H-3b3 for the m-TFMB flow path and H-3b2 and H-3b3 for the PFB flow path are 100.6 ft (30.7 m) and 87.9 ft (26.8 m), respectively.

Initial Tracer Input-Zone Dimensions

The tracer-test history was presented in Section 3.3. The tracer-injection procedure consisted of mixing the tracer in an initial volume of water, injecting the tracer-labeled volume, and injecting a second volume of water to displace the tracer-labeled water into the formation. Since the injection was of short duration, it was assumed that the tracer moved out under plug-flow conditions through the fractures only and resulted in an initial tracer input zone that was cylindrical in shape and encompassing a region dependent on the volume injected and the fracture porosity. The two fluid volumes that are injected determine the initial tracer-zone dimensions in the aquifer. Natural gradients were assumed to have a negligible effect on the initial tracer-mass distribution around the injection well. For a fracture porosity of 1.9×10^{-5} (determined during the model calibration of the m-TFMB breakthrough curve) and the respective fluid volumes injected, the initial tracer-input ring of the m-TFMB tracer surrounding well H-3b1 had inner and outer radii of 3.3 ft (1.0 m) and 5.6 ft (1.7 m), respectively, and the PFB tracer surrounding well H-3b2 had inner and outer radii of 4.9 ft (1.5 m) and 5.6 ft (1.7 m), respectively.

The input parameters discussed above are represented by a constant value for each simulation during calibration of the breakthrough curves. However, input-parameter values for different simulations are adjusted systematically, within ranges judged as reasonable, in an attempt to match the observed tracer-breakthrough curves.

3.6 Analysis of Tracer-Breakthrough Curves

From initial inspection of the two breakthrough curves (Figure 4), one can identify major differences in tracer breakthrough. The m-TFMB

curve peaks sharply early in the test, whereas the PFB curve is very broad, is of much lower concentration, and requires a significant portion of the test period to reach the maximum observed concentration. With the current double-porosity conceptualization, it was possible to achieve reasonable breakthrough-curve matches with system parameters consistent with the current physical and conceptual understanding of the Culebra. The best-fit parameters are summarized in Table 2.

The tortuosity chosen during calibration has a direct effect on the estimate of matrix-block size because tortuosity is part of the product which SWIFT II defines as molecular diffusivity (see Equation 1). Rasmuson and Neretnieks (1981) define the characteristic time for diffusion as:

$$t_c = L_m^2 / D^* \quad (4)$$

where t_c is equal to the characteristic time for diffusion; L_m is equal to one-half of the matrix-block length; and D^* is equal to the solute molecular diffusivity of the matrix. This characteristic time for diffusion in part controls the transient behavior of the breakthrough curve. Therefore, if one varies tortuosity (i.e., D^*), then one must compensate with the value of L_m to achieve the same breakthrough curve. Good fits between observed and simulated breakthrough curves were obtained for tortuosities of 0.15 and 0.45. From a literature review of tortuosities for consolidated materials, 0.15 is considered to be more appropriate. Only the results for a tortuosity of 0.15 are presented here.

Figure 6 shows the comparison of the observed and simulated breakthrough curves (concentration expressed as mass per unit mass) for the m-TFMB tracer on the H-3b1 to H-3b3 flow path for a tortuosity of 0.15. A longitudinal dispersivity of 9.8 ft (3.0 m) and a fracture

Table 2 Summary of Best-Fit Input Parameters for m-TFMB and PFB Breakthrough Curves at the H-3 Hydropad

Parameter	Tracer	
	m-TFMB	PFB
Solute free-water diffusion coefficient (ft ² /d)	6.9 x 10 ⁻⁴	6.7 x 10 ⁻⁴
(m ² /s)	7.4 x 10 ⁻¹⁰	7.2 x 10 ⁻¹⁰
Tortuosity	0.15	0.15
Matrix-block length (ft)	3.9	0.8
(m)	1.2	0.25
Longitudinal dispersivity (ft)	9.8	4.9
(m)	3.0	1.5
Fracture porosity	1.9 x 10 ⁻³	1.9 x 10 ⁻³
Matrix porosity	0.2	0.2

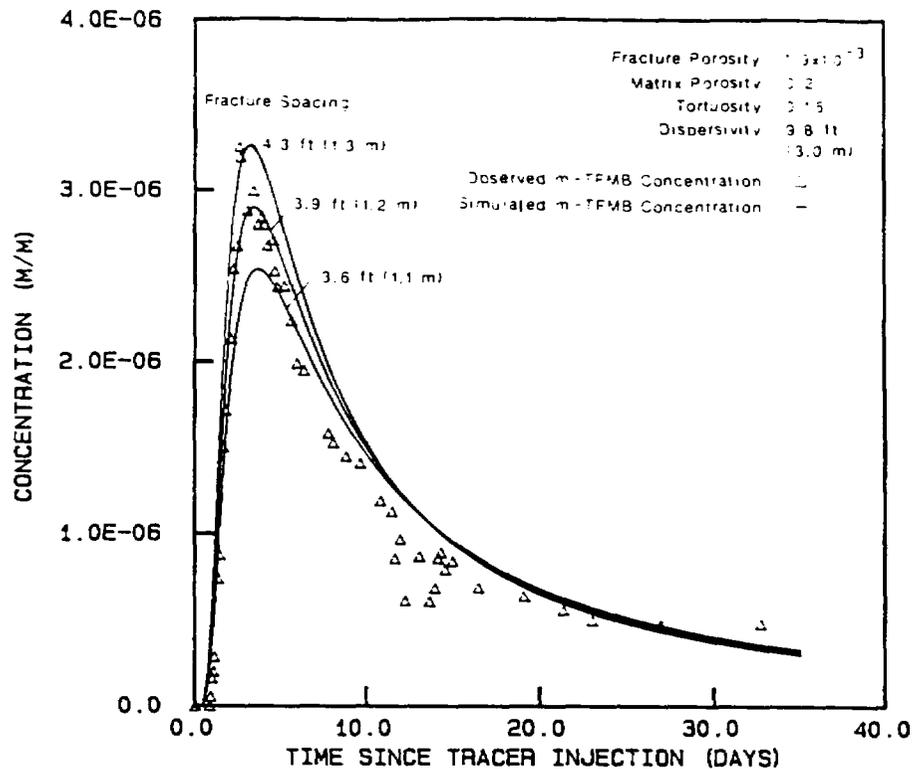


Figure 6 Observed and Simulated Breakthrough Curves for Tracer m-TFMB

porosity of 1.9×10^{-3} provided the best-fit simulated breakthrough curve. An effective matrix-block size of 3.9 ft (1.2 m) is considered representative for fitting the m-TFMB breakthrough curve. Simulated breakthrough curves for matrix-block sizes of 4.3 ft (1.3 m) and 3.6 ft (1.1 m) are also shown for comparison in Figure 6.

The observed and simulated breakthrough curves for PFB for the H-3b2 to H-3b3 flow path are shown in Figure 7 for a tortuosity of 0.15. As discussed earlier, the breakthrough curve for PFB did not indicate fracture-controlled transport. Using the same fracture porosity as for fitting the m-TFMB breakthrough curve, a dispersivity of 4.9 ft (1.5 m) and an assumed tortuosity of 0.15 resulted in an effective matrix-block size of 0.8 ft (0.25 m).

A simulation was conducted using SWIFT II with a single-porosity conceptualization for the H-3b1 to H-3b3 flow path (m-TFMB flow path) to evaluate whether or not a single-porosity model would adequately simulate the tracer-breakthrough curve. The parameter values were chosen similar to those for the double-porosity analysis of the m-TFMB breakthrough curve. A tortuosity of 0.15 and porosity of 1.9×10^{-3} were chosen. This porosity was chosen because it has the primary control on the arrival time of the peak concentration. The observed m-TFMB breakthrough curve and the simulated breakthrough curves for the single-porosity and double-porosity

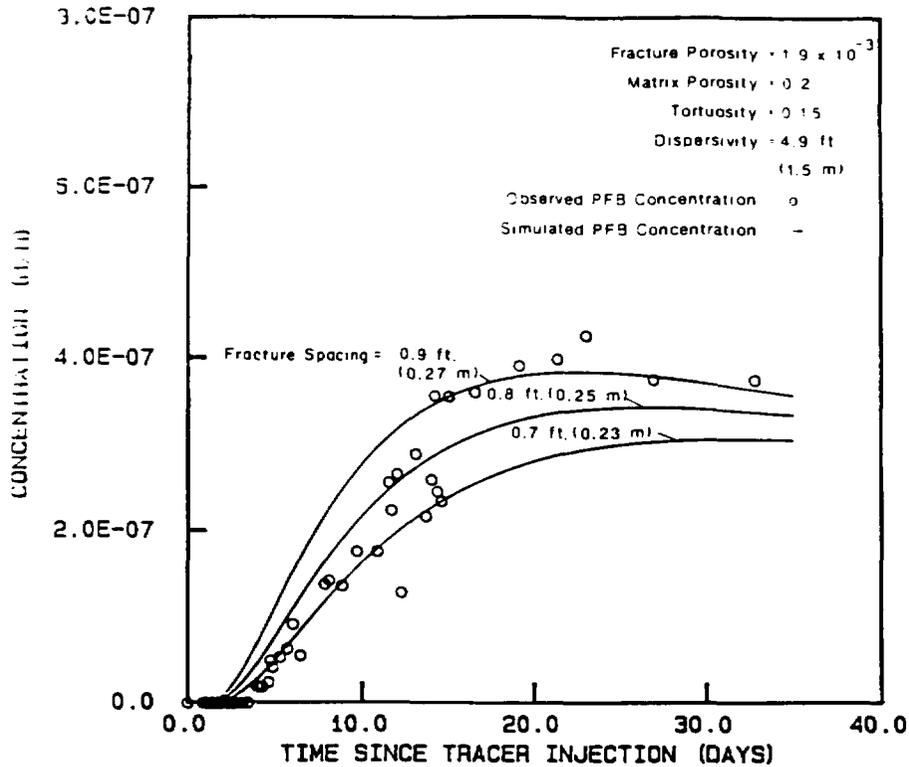


Figure 7 Observed and Simulated Breakthrough Curves for Tracer PFB

conceptualizations are shown in Figure 8. It is evident from comparison of the observed and simulated breakthrough curves that it would be difficult to obtain a single-porosity calibration of the observed tracer-breakthrough curve.

Dispersivity is defined and applied consistent with a Fickian conceptualization in the SWIFT II model. The longitudinal dispersivities obtained for the two flow paths are within a factor of two. From a sensitivity analysis (Kelley and Pickens, 1986), it was found that increasing dispersivity alone caused an earlier tracer arrival and higher peak concentration. The difference in dispersivities for the two flow paths can be viewed as a measure of either differences in heterogeneity between the two flow paths traveled by the tracers or a result of difficulties in providing a unique fit of observed and simulated breakthrough curves for processes described by such a large number of parameters.

The characteristic matrix-block sizes estimated from calibration of the breakthrough curves varied between the flow paths. The estimated block size for the H-3b1 to H-3b3 flow path is approximately 4.8 times larger than the block size estimated for the H-3b2 to H-3b3 flow path. Although the calculated matrix-block sizes are consistent with observations from core samples, shaft excavations, and outcrop areas, there are various factors which might in part explain the different

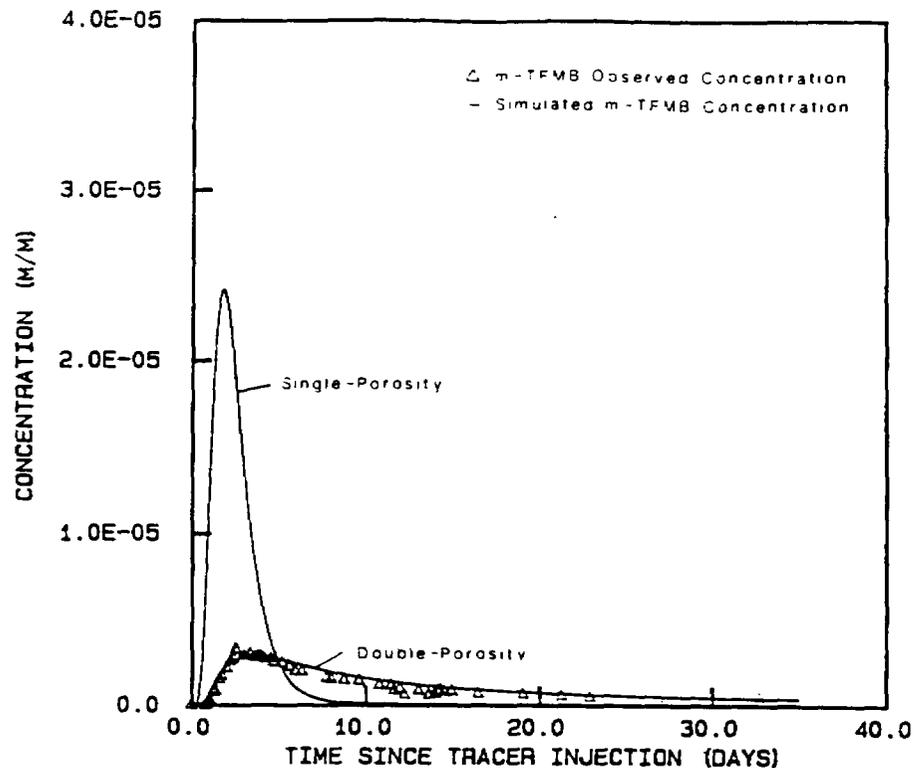


Figure 8 Comparison of Observed and Simulated Breakthrough Curves (Single- and Double-Porosity Conceptualization) for Tracer m-TFMB

matrix-block sizes calculated for the respective flow paths. Some of the possible factors are: (1) differences in tracer behavior (diffusion coefficients, sorptive characteristics, biodegradability); (2) differences in tracer-input conditions (i.e., input functions); (3) anisotropic and non-homogeneous transport characteristics of the medium; and (4) regional gradients being of significant importance relative to local gradients induced by the convergent-flow field.

Differences in tracer behavior have been shown to be minimal in laboratory free-water diffusion tests (Walter, 1982). Both tracers m-TFMB and PFB have been used for convergent-flow tracer tests in the Culebra dolomite at the H-6 hydropad. If one did suspect that these two tracers had different behavior under field conditions, one would expect their different behaviors to be similar at various tracer-test locations. In contrast, at the H-6 hydropad, m-TFMB had a very broad and low-concentration breakthrough curve while PFB had a very sharp and relatively high-concentration breakthrough curve. This implies that the breakthrough curve differences stem from flow-path differences rather than tracer-behavior differences. As mentioned in Section 3.2, both tracers should have been resistant to biodegradation over the duration of the test (Stetzenbach, personal communication).

As mentioned earlier, another potential cause for the differences in breakthrough curves is a difference in input functions at the two tracer-addition wells. If all of the tracer mass did not enter the aquifer initially, tracer could have continued to have been introduced to the aquifer from the well during the test. This condition would result in a time-dependent input function that could have an important effect on interpreting the breakthrough curves. After each of the tracer injections, a sufficient volume of water was added in order to displace the wellbore volumes completely within the first 1 to 2 hours after tracer injection. The input functions were simulated to match this input procedure. Due to a lack of information concerning wellbore concentration versus time in the tracer-addition wells, and due to the non-uniqueness of the calibrated parameters, it is not possible to assess whether some of the tracer mass may have remained in the tracer-addition wells.

The model treated the Culebra as an isotropic homogeneous medium. It is known that hydropad-scale heterogeneities exist at the H-3 hydropad through core reconnaissance. Anisotropy has been determined to be weak from hydraulic testing at other hydropads and cannot be differentiated from heterogeneities (Gonzalez, 1983). Through the analysis of two long-term pumping tests conducted at the H-3 hydropad, Beauheim (1987) found evidence for a preferential hydraulic connection between wells H-3b1 and H-3b3. If this is true, and the H-3b1 to H-3b3 (m-TFMB) flow path is more direct than the H-3b2 to H-3b3 flowpath (PFB), this could explain the broader and lower concentration breakthrough curve exhibited by PFB. This effectively means that the PFB tracer would travel a longer flow path, and since this extension of the flow path is not accounted for in the model, the matrix-block size must be decreased to compensate for the apparent increase in diffusivity or the real increase in surface area available for diffusion.

Regional hydraulic gradients range from 1×10^{-3} to 4×10^{-3} in the Culebra (Mercer, 1983). Hydraulic gradients at the H-3 hydropad during the convergent-flow tracer test are estimated to be an order of magnitude greater than the regional gradient and, therefore, would have dominated locally.

It is recognized that uncertainty exists in the assumed or calibrated values for tortuosity, fracture porosity, matrix porosity, and matrix-block size used to describe solute transport at the H-3 hydropad. Reducing this uncertainty would require additional laboratory and field testing (e.g., additional drilling and coring, additional matrix-porosity determinations on core, diffusion experiments, and additional field tracer testing). The results obtained from the conservative-tracer test indicate that fracture flow and matrix diffusion dominate solute transport in the Culebra at the H-3 hydropad. Further, the parameters derived to fit the m-TFMB and PFB breakthrough curves are thought to be consistent with current conceptualizations of the Culebra at the H-3 hydropad.

4.0 Conclusions

The following conclusions can be drawn from interpretation of a conservative-tracer test conducted at the H-3 hydropad in the Culebra Dolomite Member at the Waste Isolation Pilot Plant site:

1. The rate of transport of the tracer between the tracer-addition wells and the pumping well indicated that transport was dominated by the presence of fractures and by diffusive transport between the fractures and the matrix.
2. The tracer-breakthrough curves could be simulated by approximating the Culebra dolomite as a fractured medium with three orthogonal fracture sets. While this is an idealized representation of a natural system, it is consistent with other physical observations and provides the ability to handle the solution of double-porosity transport at the field scale as a tenable problem.
3. The interpreted matrix-block sizes for the two tracer flow paths at the hydropad were 3.9 ft (1.2 m) and 0.8 ft (0.25 m). Because of the large number of fitting parameters, uncertainty exists in the representativeness of these matrix-block sizes. However, they should be considered to be at least qualitative and to provide an indication of the fracture-fluid volume and surface area available for diffusion in order to fit the observed tracer-breakthrough curves.

The estimates of fracture porosity and effective matrix-block size are specific to the location of the tracer test. They do provide, however, initial estimates on which to base predictions of tracer transport for a proposed sorbing tracer test and for regional scale transport of solutes in the Culebra.

Acknowledgements

This work was supported by the U.S. Department of Energy under contract DE-AC04-76DP00789. This study has been improved by technical review from G. E. Grisak and G. J. Saulnier (INTERA Technologies, Inc.) and A.R. Lappin, and D. Tomasko (Sandia National Laboratories). The authors would also like to thank C. H. Lowenberg and J. E. Cramer for their care in preparing this manuscript.

Biographical Sketches

Both J.F. Pickens and V.A. Kelley are hydrogeologists with INTERA Technologies, Inc., at Austin, Texas. Research interests include the application of hydraulic and tracer testing techniques for characterizing the transport properties of porous and fractured geologic environments.

Mark Reeves is a senior staff consultant at INTERA Technologies, Inc., and holds three degrees in physics. He is perhaps best known for his development and application work with two groups of flow and transport codes: the saturated-unsaturated models now known as FEMWATER and FEMWASTE and the nuclear waste isolation models SWIFT and SWIFT II. Currently, he is working on a group of new models called SYSNET which statistically analyze human-intrusion scenarios for a nuclear waste salt-site repository.

R.L. Beauheim is a hydrogeologist with the Earth Sciences Division of Sandia National Laboratories. His background has involved the development and application of field and interpretive methodologies for characterizing fractured geologic formations. He currently directs the hydrologic investigations at the Waste Isolation Pilot Plant site.

References

- Lorenblatt, G.I., Y.P. Zheltov, and I.N. Kochina, 1960. Basic concepts in the theory of seepage of homogeneous liquids in fissured rocks (strata). *Journal of Applied Mathematics and Mechanics (USSR)*, Vol. 24, No. 5, p. 1286-1303.
- Barker, J.A. and S.S.D. Foster, 1981. A diffusion exchange model for solute movement in fissured porous rock. *QJ. Eng. Geol.*, V.14, p. 17-26.
- Bear, J., 1972. *Dynamics of Fluids in Porous Media*. American Elsevier Publishing Company, New York, 764 p.
- Beauheim, R.L., 1987. Analysis of Pumping Tests of the Culebra Dolomite Conducted at the H-3 Hydropad at the Waste Isolation Pilot Plant (WIPP) Site. Sandia National Laboratories, SAND 86-2311.
- Black, S.R., R.S. Newton, and D.K. Shukla, editors, 1983. Results of Site Validation Experiments - Volume 2 of 2. Supporting Documents 5-14. U.S. Department of Energy, TME 3177.
- Chaturvedi, L. and K. Rehfeltdt, 1984. Groundwater occurrence and the dissolution of salt at the WIPP radioactive waste repository site. *American Geophysical Union, EOS*, July 3, 1984, p. 457-459.
- Core Laboratories, Inc., 1986a. A Complete Petrographic Study of Various Samples From The Rustler Formation. Performed for INTERA Technologies, Inc., under contract for Sandia National Laboratories, Unpublished.
- Core Laboratories, Inc., 1986b. Special Core Analysis Study for INTERA Technologies, WIPP Site, File Number: SCAL 203-850073. Core Laboratories Inc., Aurora, Colorado.
- Ferrall, C.C. and J.F. Gibbons, 1980. Core Study of Rustler Formation Over the WIPP Site, Sandia National Laboratories, Contractor Report, SAND79-7110, 80 p.
- Gonzalez, D.D., 1983. Groundwater Flow in the Rustler Formation, Waste Isolation Pilot Plant (WIPP), Southeast New Mexico (SENM): Interim Report. Sandia National Laboratories, SAND82-1012, 39 p.
- Haug A., V.A. Kelley, A.M. LaVenue, and J.F. Pickens, 1987. Modeling of Ground-Water Flow in the Culebra Dolomite at the Waste Isolation Pilot Plant (WIPP) Site: Interim Report, Sandia National Laboratories, SAND86-7167.

- Haug, A., 1987. A Modeling Study of the Culebra Dolomite, paper present at the NWWA Conference "Solving Ground Water Problems with Model held February 10-12, 1987, Denver, Colorado, 26 p.
- Holt, R.M., and D.W. Powers, 1984. Geotechnical Activities in the Waste Handling Shaft, Waste Isolation Pilot Plant (WIPP) Project in Southeastern New Mexico. U.S. Department of Energy, WTSD-TME-038.
- Hydro Geo Chem, in preparation. Convergent Flow Tracer Tests at the H-Hydropad, Waste Isolation Pilot Plant (WIPP), Southeastern New Mexico (SENM). Unpublished contractor report prepared for Sandia National Laboratories, 88 p.
- INTERA Technologies, Inc., 1986. WIPP Hydrology Program, Waste Isolation Pilot Plant, Southeastern New Mexico, Hydrologic Data Report #3 Sandia National Laboratories, Contractor Report SAND 86-7109.
- Katsube, T.J., T.W. Melnyk, and J.P. Hume, 1986. Pore Structure From Diffusion in Granitic Rocks. Atomic Energy of Canada Ltd., Technical Report TR-381 28 p.
- Kelley, V.A., and J.F. Pickens, 1986. Interpretation of the Convergent-Flow Tracer Tests Conducted in the Culebra Dolomite at the H-3 and H-4 Hydropads at the Waste Isolation Pilot Plant (WIPP) Site, Sandia National Laboratories, Contractor Report SAND86-7161.
- Lallemant-Barres, A. and P. Peaudecerf, 1978. Recherche des Relations Entre la Valeur de la Dispersivite Macroscopique d'un Milieu Aquifere, Ses Autres Caracteristiques et les Conditions de Mesure. Bull.Bur. Geol. Minieres (Fr.) Sect. 3, 4:277.
- Mercer, J.W., 1983. Geohydrology of the Proposed Waste Isolation Pilot Plant Site, Los Medanos Area, Southeastern New Mexico. U.S. Geological Survey Water-Resources Investigation Report 83-4016, 113 p.
- Neretnieks, I., 1972. Analysis of some washing experiments of cooked chips, Sven. Papperstidn., 75, p. 819.
- Neretnieks, I., 1980. Diffusion in the rock matrix: An important factor in radionuclide retardation?, J. Geophys. Res., 85, p. 4379.
- Pickens, J.F. and G.E. Grisak, 1981. Scale-dependent dispersion in a stratified granular aquifer. Water Resources Research, V.17, No. 4, p. 1191-1211.
- Rasmuson, A. and I. Neretnieks, 1981. Migration of radionuclides in fissured rock: The influence of micropore diffusion and longitudinal dispersion, J. Geophys. Res., 86, p. 3749-3758.
- Rasmuson, A, T.N. Narasimhan, and I. Neretnieks, 1982. Chemical transport in a fissured rock: Verification of a numerical model. Water Resources Research V.18, No. 5, p. 1479-1492.

- Reeves, M., N.D. Johns, and R.M. Cranwell, 1986. Theory and Implementation for SWIFT II, Sandia Waste-Isolation Flow and Transport Model for Fractured Media, Release 4.84. Sandia National Laboratories, NUREG/CR-3328 and SAND83-1159.
- Reinfeldt, K., 1984. Sensitivity Analysis of Solute Transport in Fractures and Determination of Anisotropy Within the Culebra Dolomite. New Mexico Environmental Evaluation Group, EEG-27.
- Raulnier, G.J., Jr., G.A. Freeze, and W.A. Stensrud, 1987. WIPP Hydrology Program, Waste Isolation Pilot Plant, Southeastern New Mexico, Hydrologic Data Report #4. Sandia National Laboratories, Contractor Report SAND86-7166.
- Stetzenbach, K.J., S.L. Jensen, and G.W. Thompson, 1982. Trace Enrichment of Fluorinated Organic Acids Used as Ground-Water Tracers by Liquid Chromatography. Environmental Science and Technology, V.16, p. 250-254.
- Streltsova-Adams, T.D., 1978. Well Hydraulics in Heterogeneous Aquifer Formations, Advances in Hydrosciences, V.T. Chow ed., V.II, New York, New York, p. 357-423.
- Vine, J.D., 1963. Surface Geology of the Nash Draw Quadrangle, Eddy County, New Mexico. U.S. Geological Survey Bulletin 1141-B, 46 p.
- Walter, G.R., 1982. Theoretical and Experimental Determination of Matrix Diffusion and Related Solute Transport Properties of Fractured Tuffs from the Nevada Test Site. Los Alamos National Laboratories, LA-9471-MS, 132 p.

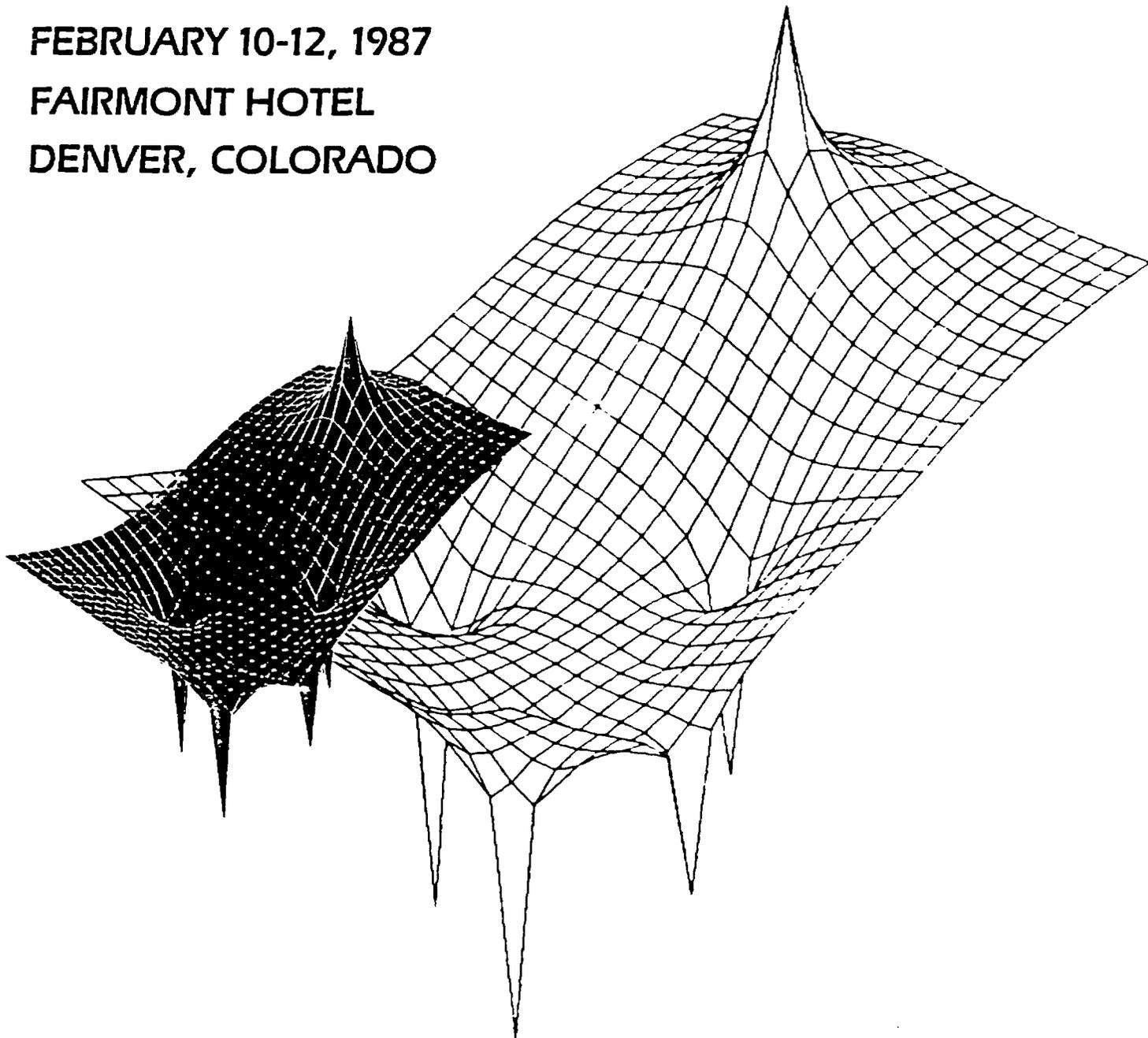
SOLVING GROUND WATER PROBLEMS WITH MODELS

*An intensive three-day conference and exposition devoted
exclusively to ground water modeling*

FEBRUARY 10-12, 1987

FAIRMONT HOTEL

DENVER, COLORADO



Sponsored by

**The Association of Ground Water Scientists and Engineers
(A Division of the National Water Well Association)**

International Ground Water Modeling Center, Holcomb Research Institute