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Representation of Spatial Variability for Modelling of Flow and Transport Processes in the Culebra Dolomite at the WIPP Site

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Abstract

The Waste Isolation Pilot Plant (WIPP) is a proposed repository for transuranic wastes constructed in bedded Permian-age halite deposits in southeastern New Mexico, USA. Site-characterization studies at the WIPP site identified groundwater flow in the Culebra Dolomite Member of the Rustler Formation as the most likely geologic pathway for radionuclide transport to the accessible environment in the event of a breach of the WIPP repository through inadvertent human intrusion. The Culebra is a 7-m-thick, variably fractured dolomite with massive and vuggy layers. Detailed studies at all scales demonstrated that the Culebra is a heterogeneous medium.

Heterogeneity in Culebra properties was incorporated into numerical simulations used for data interpretation and PA calculations in different ways, depending on the amount of data available, the certainty with which the effects of a given approach could be evaluated, and the purpose of the study. When abundant, spatially distributed data were available, the heterogeneity was explicitly included. For example, a stochastic approach was used to generate numerous, equally likely, heterogeneous transmissivity fields conditioned on head and transmissivity data. In other cases, constant parameter values were applied over the model domain. These constant values were selected and applied in two different ways. In simple cases where a conservative bounding value could be identified that would not lead to unrealistically conservative results, that value was used for all calculations. In more complex cases, parameter distributions were developed and single values of the parameters were sampled from the distributions and applied across the entire model domain for each of the PA Monte Carlo simulations. We are currently working to refine our understanding of the multiple rates of diffusion attributable to small-scale spatial variability. We hope to define a distribution of diffusion rates that can be used directly, or in simplified form, to represent the diffusion process more accurately at the PA scale.

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Introduction

The Waste Isolation Pilot Plant (WIPP) is a proposed repository for transuranic wastes constructed in bedded Permian-age halite deposits in southeastern New Mexico, USA (Figure 1). Site-characterization studies at the WIPP site identified groundwater flow in the Culebra Dolomite Member of the Rustler Formation as the most likely geologic pathway for radionuclide transport to the accessible environment in the event of a breach of the WIPP repository through inadvertent human intrusion. The Rustler Formation represents the transition between the underlying thick evaporite beds of the Salado Formation (where the WIPP repository has been excavated) and the overlying clastic-dominated continental deposits of the Dewey Lake Redbeds. In the vicinity of the WIPP site, the Culebra is the most transmissive unit in the Rustler Formation.

The Culebra is a 7-m-thick, variably fractured dolomite with massive and vuggy layers. The Culebra is underlain by a mudstone unit and overlain by an anhydrite unit [1]. Over the last 20 years, many studies have been conducted on the Culebra geology and on flow and transport processes. These studies have included: geologic studies of core, shafts, and outcrops; measurements of core permeability, porosity, and formation factor; single- and multi-well hydraulic tests; single- and multi-well tracer tests of physical transport processes; laboratory diffusion tests; batch and core tests of chemical processes and properties; and both two- and three-dimensional regional groundwater flow modelling. The insights gathered from interpretation of data and numerical modelling have formed the basis for a detailed conceptual model of Culebra flow and transport processes. To apply data from laboratory and

field observations to performance assessment (PA), the conceptual model must include an understanding of processes and their dependence on both temporal and spatial scales.

Background

Detailed studies at all scales demonstrated that the Culebra is a heterogeneous medium. Within the 41.4 km² area of the WIPP site, 44 wells and four shafts penetrate the Culebra (Figure 2), which is located about 230 m below land surface. Hydraulic tests have demonstrated that the transmissivity of the Culebra varies over at least six orders of magnitude in the vicinity of the WIPP site (Figure 2) [2]. Tracer tests at several sites suggest that transport properties also vary significantly. Detailed examination of core and shaft exposures suggests that multiple scales of porosity are present within the Culebra, including fractures ranging from

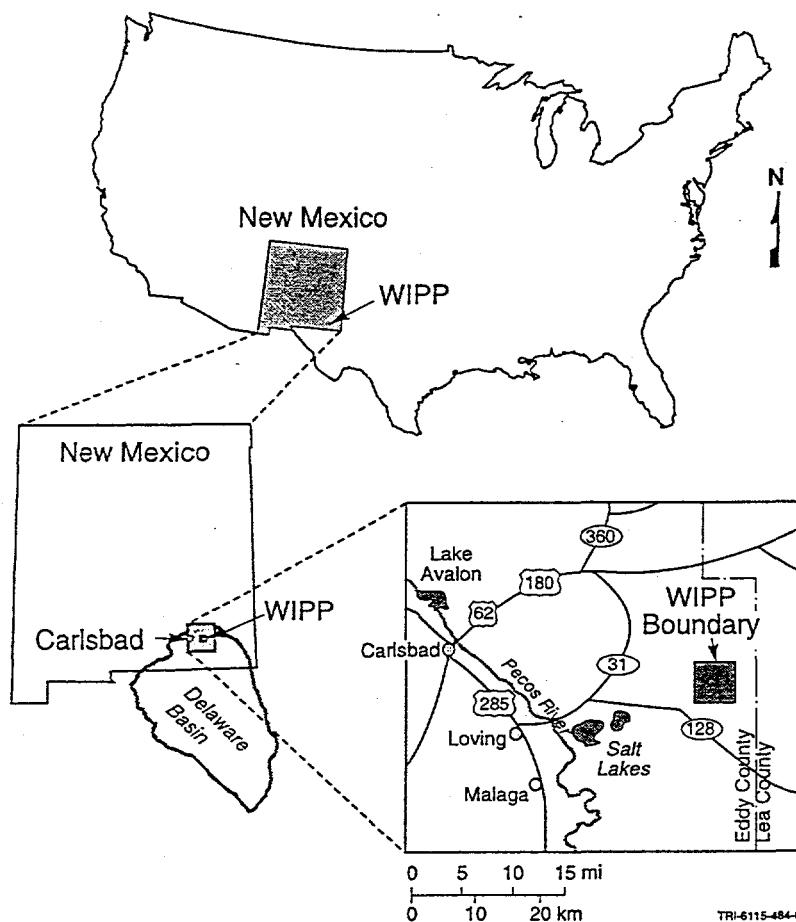


Figure 1. Location of the WIPP site

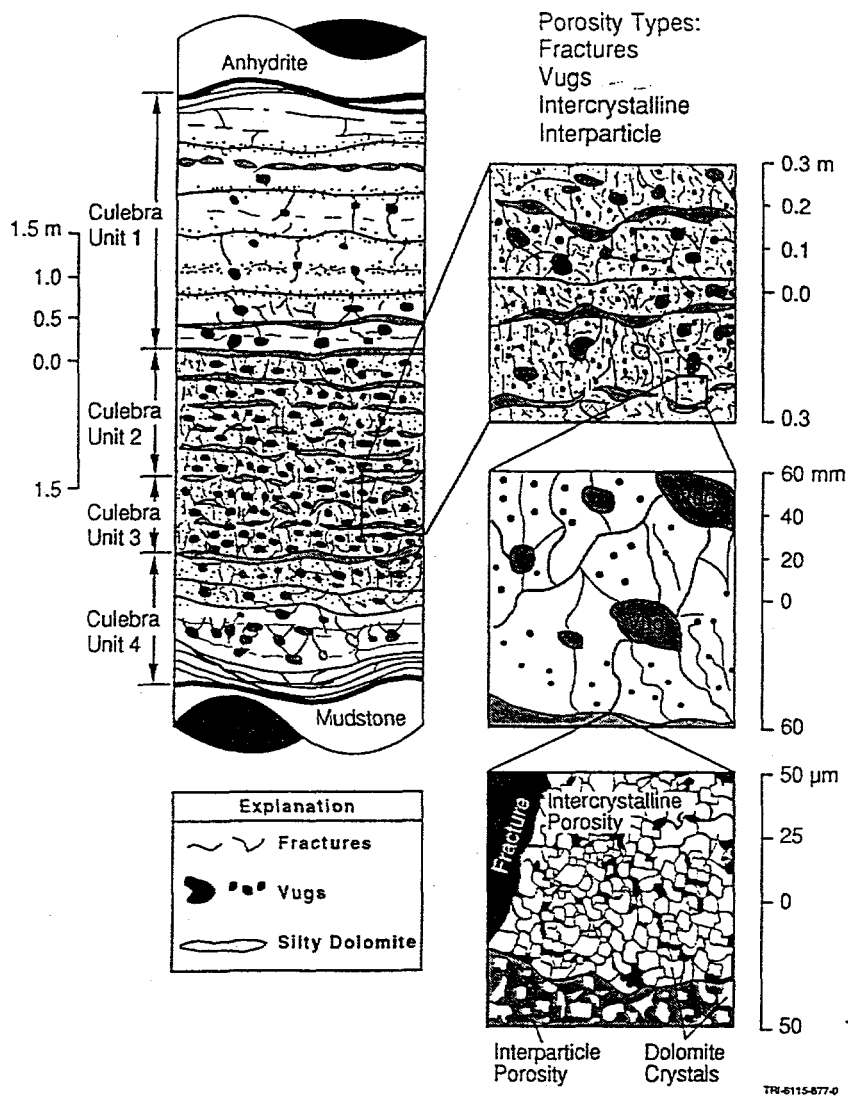


Figure 3. Schematic of Culebra units and porosity types

Modelling of Heterogeneity

Heterogeneity was incorporated into numerical simulations used for data interpretation and PA calculations in different ways, depending on the amount of data available, the certainty with which the effects of a given approach could be evaluated, and the purpose of the study. In some cases, the heterogeneity was explicitly included. For example, stochastic approaches were used to generate heterogeneous (conditioned or unconditioned) fields of transmissivity for flow and transport calculations at different scales. In other cases, a constant parameter value was selected in one of two ways and applied over the model domain. If a conservative bounding value could be identified that would not lead to unrealistically conservative results, that value was used for all calculations. If a bounding value could not be used without producing unrealistic results, a parameter distribution was de-

veloped and a single value of the parameter was sampled from the distribution and applied across the entire model domain for each of the PA Monte Carlo simulations. These approaches are discussed below in relation to several Culebra flow and transport numerical modelling activities.

The first example is a brief overview of the generation of heterogeneous transmissivity (T) fields for the WIPP Compliance Certification Application (CCA) [7]. To represent the heterogeneity in flow and transport simulations, 100 T-field realizations were generated and sampled on for the PA Monte Carlo simulations. The objective of this modelling activity was to take the available hydraulic data (including estimated measurement uncertainties) and generate numerous equally likely calibrated T fields, each with different spatial characteristics. The T fields were generated using an automated inverse code, GRASP-INV, that uses pilot points (synthetic measured-transmissivity locations) to improve the model fit to the data until acceptance criteria are met. This method is a refinement of the method used for the 1992 PA [8]. The initial information for the T fields came from the transmissivities and steady-state hydraulic heads measured at individual wells across the WIPP site area. The T fields were calibrated by comparing simulated responses to the observed transient pressure/water-level

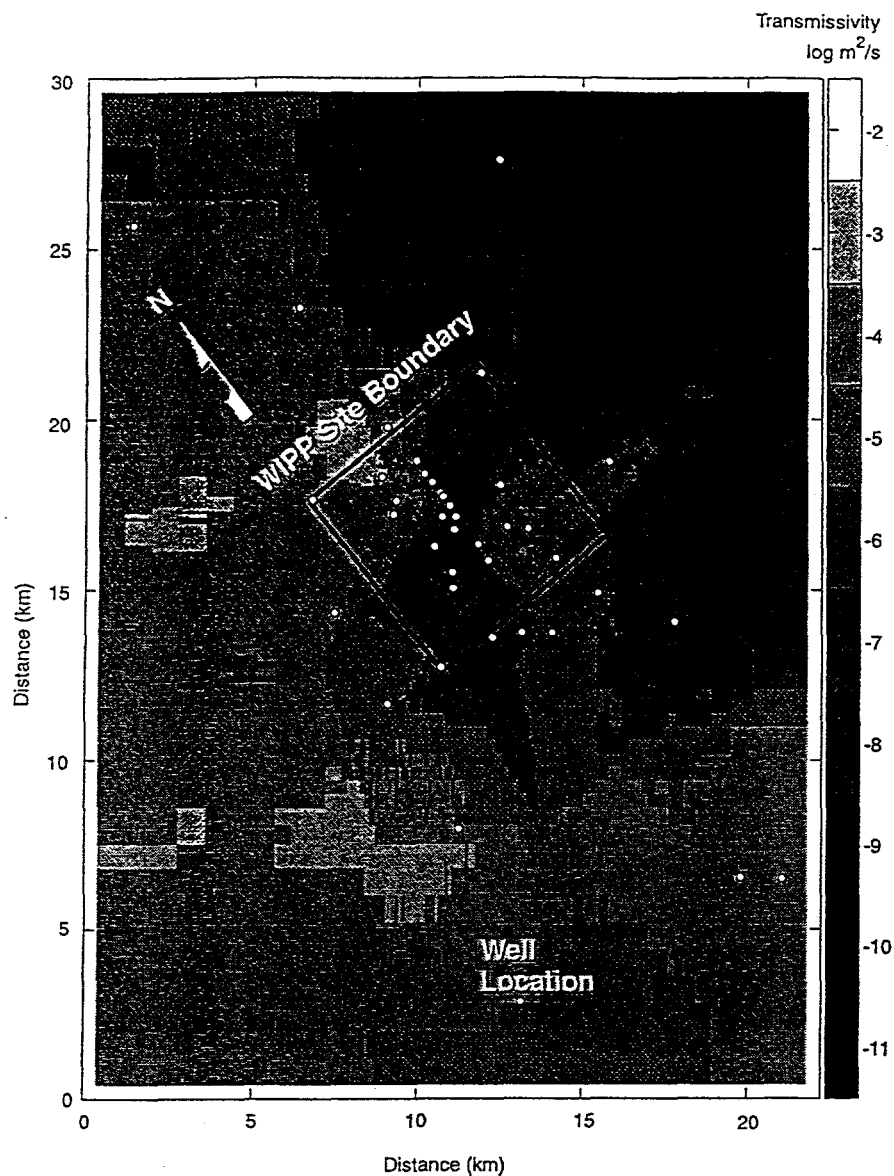


Figure 4. The ensemble average of all 100 T fields

was treated by excluding CU 1 from consideration and using a constant Culebra thickness of approximately 4 m, representing the average thickness of CU 2-4, in all transport calculations. This is a conservative approach because it reduces the advective porosity, thereby increasing the mean pore velocity, and reduces the diffusional porosity that acts to retard transport. The conservatism of this approach, however, is not thought to be grossly unrealistic such that it would obscure the importance of other parameters.

A third example of treating heterogeneity involves a set of numerical simulations of tracer tests conducted in the Culebra and the scaling of the parameters interpreted from these simulations for PA calculations. Data sets used for the numerical simulations consist of multi-well convergent-flow tracer tests conducted at the H-3 and H-11 hydropads in the 1980s and both single-well injection-withdrawal (SWIW) and multi-well convergent-flow tests conducted in 1995-96 at the H-11 and H-19 hydropads (Figure 2). The more recent tests benefited from numerous refinements, including

responses resulting from large-scale pumping tests of several months' duration and leakage into the WIPP shafts. Figure 4 shows the ensemble average of all 100 T fields. Figure 5 shows a more detailed view of one of the 100 T fields (no. 77).

Particle-tracking simulations were used to compare the 100 T fields on the basis of travel time. Particles were tracked from the location of a hypothetical intrusion borehole to the boundary of the WIPP site. The particle transport times varied by over two orders of magnitude because different T fields can have significantly different off-site transport pathways (Figure 6) and because similar pathways can have different transmissivities in different realizations.

Heterogeneity caused by differences between the properties of different Culebra layers and by variations in the thickness of the Culebra

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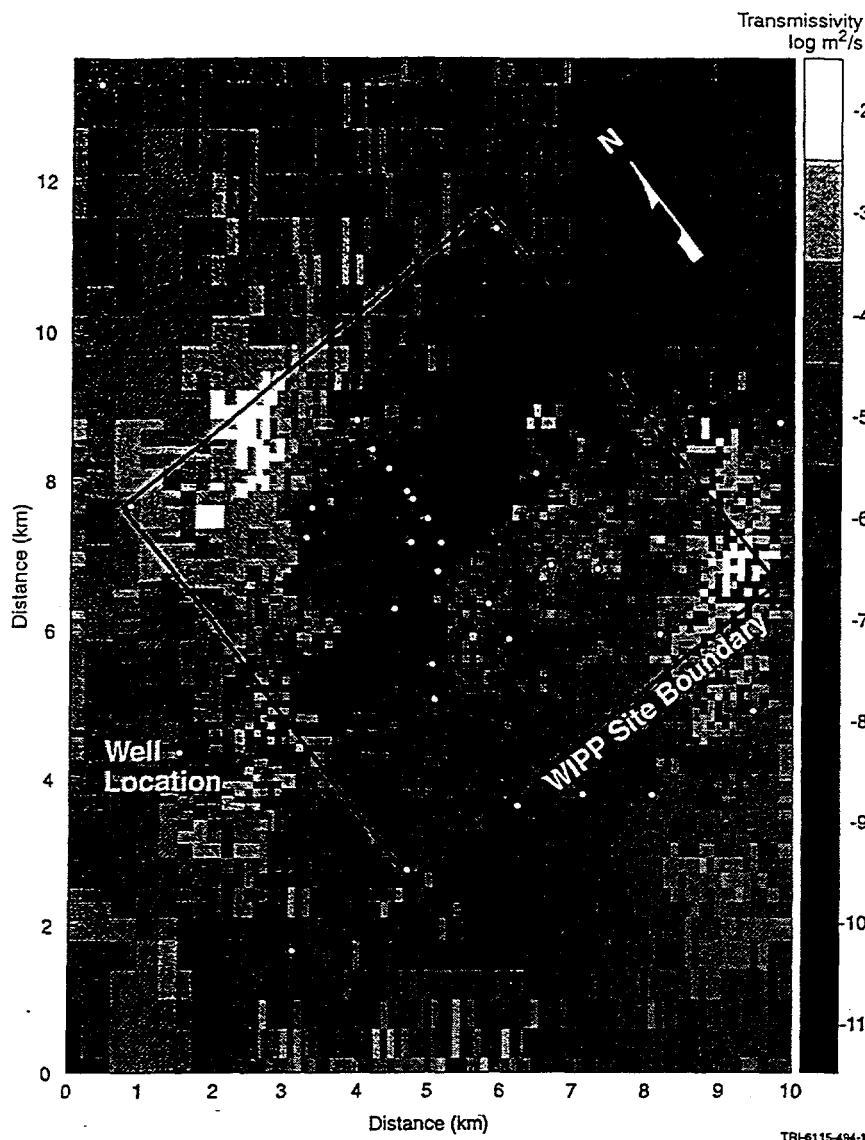


Figure 5. Example of a transient-calibrated transmissivity field (no. 77)

and were not intended to be an accurate representation of the actual spatial variability in hydraulic conductivity between wells. Interpretations of the SWIW tests indicate that the slow mass recovery observed cannot be explained by heterogeneity alone in a single-porosity ("fracture" only) conceptualization. The slow mass recovery would be expected, however, if diffusional mass-transfer between advective and non-advective porosity were controlling tracer recovery (Figure 7). Simulations of the multi-well data also suggest that the data cannot be modelled adequately without "matrix" diffusion [10].

Interpretations of the SWIW tests alone cannot be used to determine unique parameter fits because a recovery curve from a SWIW test is relatively insensitive to advective porosity (Figure 7), unlike a tracer-breakthrough curve from a multi-well test. The numerical simulations of the multi-well test data were used to bracket the appropriate values for both advective porosity and mass-transfer rate (matrix-block size was used as the fitting parameter and tortuosity was held constant). Some parameters (e.g., diffusive porosity, formation thickness, mass injected) were assumed constant based on lab or field data or literature values after the sensitivity of the model to those assumed values was evalu-

repeated injections with different pumping rates at the central well and discrete injections into the upper and lower portions of the Culebra [9]. Objectives of the numerical simulations were to test the conceptual model of transport in the Culebra and interpret the tracer-test data to evaluate both the appropriate conceptual model and parameters for numerical simulations at both the tracer-test and PA scales.

Interpretations of the tracer-test data were conducted with both single- and double-porosity models. Spatial variability was incorporated into some of the simulations by generating heterogeneous, unconditioned, random fields of hydraulic conductivity at the tracer-test scale. The generated hydraulic-conductivity fields were intended to evaluate the effects the maximum plausible heterogeneity might have on the tailing in the breakthrough curves

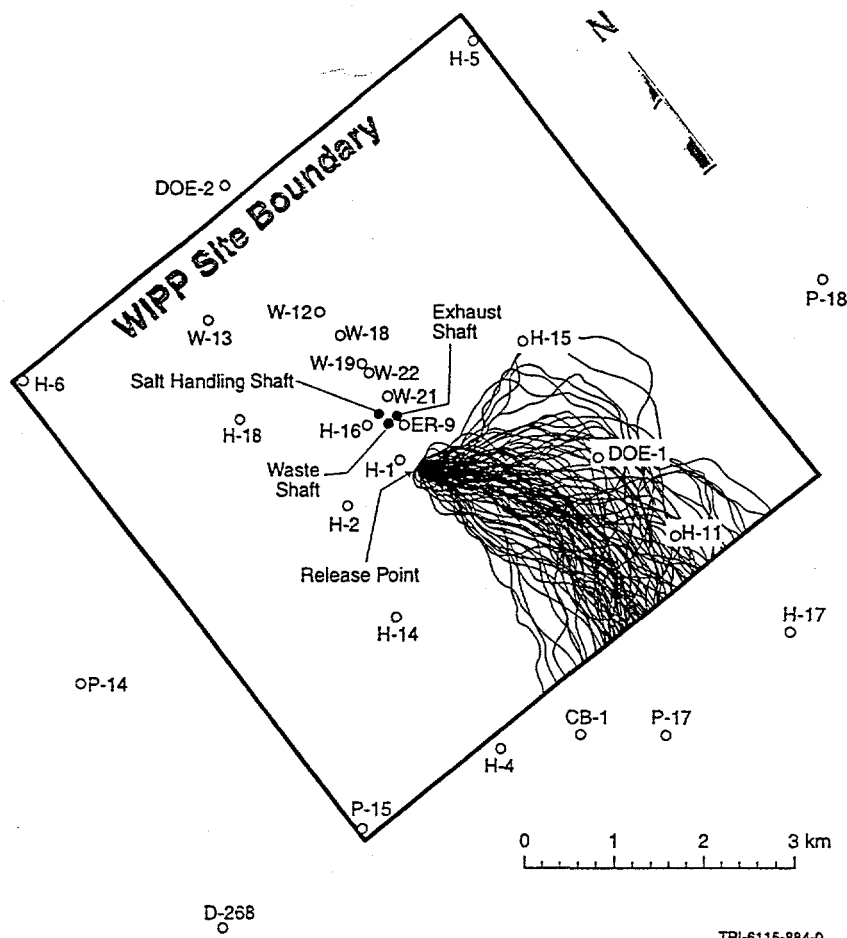


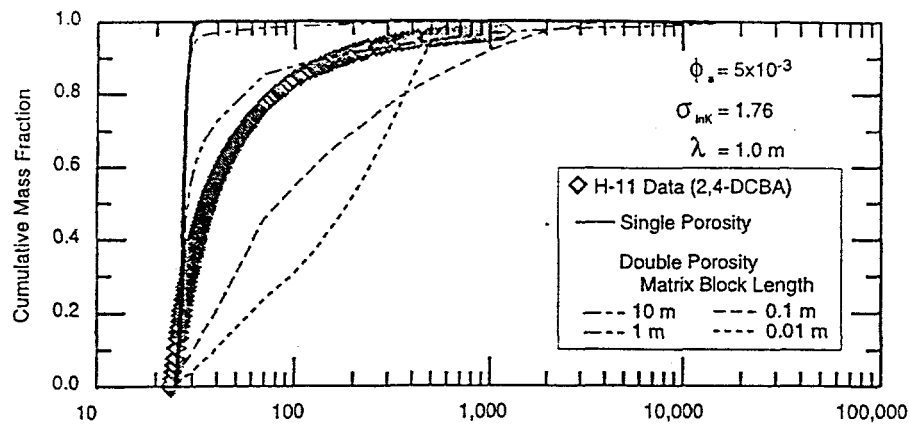
Figure 6. Travel paths corresponding to different T-field realizations

intended to represent a conservatively low range of possible effective advective-porosity values across the entire off-site pathway consistent with the tracer-test results. Other transport parameters, such as matrix-block length and diffusive porosity, were also represented by parameter distributions from which single values of the parameters were sampled and applied across the entire model domain for each Monte Carlo simulation.

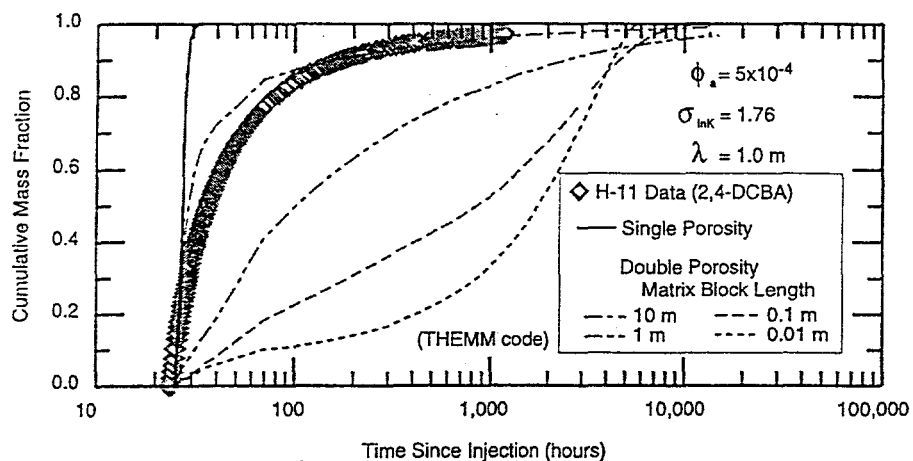
Both the PA calculations and the simulations of tracer-test data used to determine parameters employed a double-porosity model with a single rate of diffusion. Detailed modelling of the tracer-test data suggested that they are better described by a double-porosity model that incorporates multiple rates of diffusion [10]. Geologic descriptions and examination of Culebra core suggest that the spatial variability in porosity, variations in fracture spacing, and the tortuous nature of the pore space should result in significant variations in diffusion rates over relatively small volumes. Numerical simulations are being conducted with a double-porosity multirate model to evaluate the distributions of diffusion rates that best fit the tracer-test data and the significance of those distributions for the PA model. When properly implemented, the multirate model should provide a more direct method to transfer transport information between laboratory, field, and PA scales, allowing a more accurate representation of the diffusion process at the PA scale. This increased accuracy could provide a defensible basis for significant PA-model simplification, if desired.

ated. The fitted-parameter ranges were found to be relatively insensitive to heterogeneity. The determined ranges were similar for simulations with both homogeneous and heterogeneous double-porosity models.

The tracer-test simulations were used as the basis for identifying distributions for some of the transport parameters used in the Monte Carlo simulations employed for the PA calculations. Whereas spatial variability in advective transport was represented directly by the T fields as described above, spatial variations in advective porosity were not directly represented. Instead, for each PA realization, a single advective-porosity value was sampled from a distribution and applied across the entire model domain. The selected distribution (log uniform between 10^{-2} and 10^{-4}) was



(a)



(b)

Figure 7. Simulated mass recovery curves for H-11 SWIW test with single-porosity and double-porosity models compared to observed data. For the simulations, the advective porosity (ϕ_a) was 5×10^{-3} in (a) and 5×10^{-4} in (b). The heterogeneous field of hydraulic conductivity had a standard deviation (σ) in natural log space of 1.76 m/s and an exponential model with a correlation length (λ) of 1.0 m

during tracer tests, leaving diffusion between advective and non-advective porosity as the most likely explanation. Tracer-test simulations were used to define ranges of different important transport parameters, and individual values were sampled from each range for each of the PA Monte Carlo simulations.

Interpretations of the recent tracer tests have resulted in a refined conceptual model of transport in the Culebra and the demonstration that transport is not limited to fractures. Our modelling to date has adequately defined parameters for use in the PA calculations. We recently initiated a series of laboratory diffusion experiments to examine the variability in diffusion rates due to porosity variations. These laboratory experiments, in combination with descriptive information from core samples and the tracer-test data, will be used to refine our understanding of the multiple rates of diffusion attributable to small-scale spatial variability. We hope to define a distribution of diffusion rates that can

Summary

We have been successful in incorporating heterogeneity in Culebra transmissivity, thickness, and transport properties in PA models. Heterogeneity in Culebra transmissivity was incorporated by generating numerous, equally likely, heterogeneous transmissivity fields and then using a different field for each PA Monte Carlo simulation. Heterogeneity arising from differences between the properties of different Culebra layers and from variations in Culebra thickness was addressed by eliminating the low-permeability upper Culebra (CU 1) from transport models and using a constant, reduced value for thickness, resulting in conservative estimates of radionuclide transport. The effects of heterogeneity in Culebra hydraulic conductivity were found to be inadequate in explaining slow tracer recoveries

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be used directly, or in simplified form, to represent the diffusion process more accurately at the PA scale.

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