DEVELOPMENT AND APPLICATION OF A MODEL TO SIMULATE SATURATED ZONE TRANSPORT FROM THE LOCATION OF THE PROPOSED REPOSITORY FOOTPRINT AT YUCCA MOUNTAIN

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ABSTRACT

This report documents the development and application of a three-dimensional model to simulate solute transport through the saturated zone in the Yucca Mountain region. The model coupled groundwater flow fields for the Yucca Mountain region that were generated using a calibrated groundwater flow model (Winterle, 2003) with a groundwater solute transport model based on the computer code MT3DMS. The solute transport model currently simulates the transport of a conservative solute; however, the transport of nonconservative solutes can be accommodated. The model was used to simulate potential solute transport over a 10,000-year period from the vertical projection of the repository footprint at the water table to the regulatory compliance boundary located approximately 18 km [11.2 mi] down the hydraulic gradient from the repository footprint. The objectives of the simulations were to (i) gain insights into the processes and features that control the migration and spreading of solute plumes along the potential transport pathway and (ii) quantify a range of plume dimensions that may occur at the regulatory compliance boundary over a period of 10,000 years. To support the objectives of the study, several scenarios were considered. These included (i) assuming a source-size equivalent to the repository footprint to obtain the maximum plume size at the regulatory compliance boundary and (ii) assuming multiple small sources distributed across the repository footprint to determine the potential for multiple small dispersed plumes to cross the regulatory compliance boundary. Assuming a relative concentration cut-off of 10^{-3}, the results from the study indicate that plumes crossing the regulatory compliance boundary may range in width from several hundred meters to greater than 4 km [2.5 mi] and may attain depths greater than 600 m [1,969 ft]. The annual groundwater flow rate through a vertical cross section of these plumes is generally less than 2.5×10^6 m^3/yr [2,000 acre-ft/yr]. The results also indicate that small plumes migrating from opposite ends of the repository are generally focused through a narrow region south of the repository and, as a result, there appears to be no potential for distinct, widely spaced small plumes at the location of the regulatory compliance boundary. The simulations also provide information to constrain the length of the transport pathway in the tuff and valley-fill hydrostratigraphic units. Insights gained from these simulations will support review of the U.S. Department of Energy license application.

Reference:

Winterle, J. “Evaluation of Alternative Concepts for Saturated Zone Flow: Effects of Recharge and Water Table Rise on Flow Paths and Travel Times at Yucca Mountain.” San Antonio, Texas: CNWRA. 2003.

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: No original data were generated from the analyses presented in this report.

ANALYSES AND CODES: The groundwater velocities used to support the solute transport calculations in this report were based on the groundwater flow simulation model previously developed by CNWRA (Winterle, 2003). The MT3DMS Version 4.5 (Zheng and Wang, 1999) included in GMS Version 5.1 (Environmental Modeling Research Laboratory, 2005) was used to construct and execute the solute transport simulations documented in this report. The GMS interface and the MT3DMS solute transport code were validated in accordance with CNWRA Technical Operating Procedure (TOP)–18. CNWRA maintains three user licenses for GMS Version 5.1, which contain all codes and documentation. All input and output files for the groundwater flow and solute transport simulations presented in this report are documented in CNWRA Scientific Notebooks 728E and 735.

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1 INTRODUCTION

Yucca Mountain, Nye County, Nevada, is being evaluated by the U.S. Department of Energy (DOE) as a potential location for a high-level waste repository. The current DOE design has the waste emplaced in drifts located in thick unsaturated tuff deposits located approximately 300 m [984 ft] below ground surface and approximately 300 m [984 ft] above the water table. The DOE design assumes that engineered and natural barrier systems will isolate waste in the repository from the accessible environment.

The saturated zone in the Yucca Mountain region provides a pathway along which radionuclides may migrate away from the repository before entering the accessible environment should the engineered barrier systems at the repository degrade. Within the saturated zone, and in particular the saturated alluvium, it is assumed that radionuclide transport will be significantly retarded due to sorption processes before reaching the regulatory compliance boundary. Retardation will increase the time it takes each radionuclide species to reach the regulatory compliance boundary. This increase in travel time to the regulatory compliance boundary, and the associated radionuclide decay, can result in a decrease in the peak concentration of each radionuclide species at the regulatory compliance boundary. Because radionuclide concentrations at the regulatory compliance boundary are sensitive to the transport properties of the saturated zone, the saturated zone is included as part of the natural barrier system for the proposed repository, and radionuclide transport in the saturated zone is included in the DOE total system performance assessment analyses.

The saturated zone radionuclide transport abstraction model that DOE is considering for TSPA-LA[1] will likely be based on the DOE saturated zone site-scale groundwater and transport models (Bechtel SAIC Company, LLC, 2004). The abstraction model is based on the Finite Element Heat and Mass Transfer Code Version 2.20 (Lawrence Livermore National Laboratory, 2003) and includes advection along groundwater stream tubes, a random walk methodology to simulate dispersion, retardation due to sorption, and matrix diffusion.

The U.S. Nuclear Regulatory Commission (NRC) will review the license application that DOE submits to support the construction and operation of a high-level waste repository at Yucca Mountain. This review will be conducted in accordance with the guidelines outlined in the Yucca Mountain Review Plan (NRC, 2003). An evaluation of the approach DOE used to incorporate radionuclide transport in the saturated zone into their safety analysis for the repository will be included in this review. The evaluation will ensure that (i) the DOE abstraction of radionuclide transport processes contained in TSPA-LA is supported by available data, (ii) data and modeling uncertainties are appropriately considered, and (iii) reasonable alternative conceptual models are considered. The importance of transport process in the saturated zone to dose has been evaluated by NRC as part of their sensitivity analysis studies and risk insights analyses. The NRC total system performance assessment sensitivity analyses indicate that saturated alluvium length and radionuclide sorption are among the top 10 parameters that control dose (Mohanty, et al., 2002). In addition, the NRC review will ensure that the DOE demonstration of its compliance with the Individual Protection Standard and the Ground Water Protection Standard considers realistic radionuclide plumes that may migrate through the

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[1]It should be noted that Total System Performance Assessment—License Application (TSPA-LA) is referenced frequently throughout this report; consequently, the acronym TSPA-LA will be used.

saturated zone and reach the regulatory compliance boundary approximately 18 km [11.2 mi] south of Yucca Mountain.

To support a better understanding of solute transport processes in the Yucca Mountain region, the CNWRA staff developed a three-dimensional groundwater flow and solute transport model. The groundwater component of the model has been previously described by Winterle, et al. (2002) and Winterle (2003). As a first step to simulating potential radionuclide transport from the repository, a solute transport model capable of simulating the transport of a conservative solute from the repository footprint projected to the water table (hereafter referred to as the repository footprint) has been coupled to the groundwater flow model presented in Winterle (2003). This conservative solute transport model is described in this report. In addition to describing the transport model, this report also describes simulations that examine the sensitivity of the migrating plume geometry at the location of the regulatory compliance boundary to source location and aquifer properties. In particular, the simulation results showed that (i) under present-day groundwater flow conditions plumes several kilometers wide and extending more than 600 m [1968 ft] below the water table may cross the regulatory compliance boundary, (ii) the present-day annual groundwater flow rate at the location of the regulatory compliance boundary through the largest plumes simulated was less than 2.5×10^6 m^3/yr [2,000 acre-ft/yr], and (iii) although small plumes may migrate from the footprint of the potential repository, the current model does not support distinct, widely dispersed small plumes crossing the regulatory compliance boundary. Insights from these simulations may be used to (i) evaluate abstractions and models used to support the DOE Total System Performance Assessment—License Application code, (ii) support review of DOE compliance with appropriate regulatory standards (e.g., the Individual Protection Standard and the Groundwater Protection Standard), and (iii) provide insights for possible future modeling studies of saturated zone radionuclide transport models for the Yucca Mountain region.

Section 2 of this report summarizes the implementation of the saturated zone solute transport model developed for the Yucca Mountain region. The results of simulations to evaluate various solute transport scenarios are described in Section 3. A summary of the findings of this work along with recommendations for future work are summarized in Section 4.

The TPA Version 5.0.1 code software validation has not been completed. The use of parameter ranges from the code, therefore, represent current unofficial best estimates that may change in the official release of the code.

2 OVERVIEW OF THE MODELING APPROACH

2.1 Introduction

Solute transport modeling often involves coupling a groundwater flow model to a mass transport model. In this coupled framework, the groundwater flow model is used to compute the velocity field that is used to model advection, dispersion, and source/sink processes represented in the mass transport model. This section of the report summarizes the coupling saturated zone groundwater flow and the mass transport models to simulate potential solute migration from the location of the proposed high-level waste repository footprint to the regulatory compliance boundary located 18 km [11.2 mi] away.

Note that the figures described in this section of the report are located at the end of this section.

2.2 Groundwater Flow Model

The groundwater model described in Winterle (2003) is based on the modular finite-difference groundwater flow modeling package MODFLOW-96 (Harbaugh and McDonald, 1996) included in the GMS Version 3.1 (Environmental Modeling Research Laboratory, 1999). The model was subsequently tested (Winterle, 2005) with the MODFLOW-2000 code (Harbaugh, et al., 2000), which was executed using the GMS Version 5.1 (Environmental Modeling Research Laboratory, 2005) user interface. Both MODFLOW-96 and MODFLOW-2000 are based on a finite difference approximation applied to the continuity equation describing groundwater flow in a single continuum heterogeneous medium.

The Yucca Mountain simulation domain described by Winterle, et al. (2002) and Winterle (2003) is 28.5 km [17.7 mi] east-west, 41.4km [25.7 mi] north-south, and 2.7 km [1.7 mi] in vertical extent (Figure 2-1; c.f., Winterle, 2003, Figure 2-1). The simulation model domain was divided into 95 columns and 138 rows in the horizontal plane to produce 13,110 grid cells with the x and y dimensions of each cell being $\Delta x = \Delta y = 300$ m [984 ft]. In the vertical direction, the model was divided into 30 horizontal layers that varied in thickness from 50 m [164 ft] to 200 m [656 ft], with the thinnest layers located near the water table. The complete discretization produced 393,300 finite difference grid cells. Only a subset of these cells were used in the MODFLOW computations, as cells located in the unsaturated zone above the water table were not considered to be part of the computational domain. The top of the active grid was determined within MODFLOW by using the confined/unconfined solution option. Estimates of the hydraulic head derived from the water table map of Winterle, et al. (2002) were used to define Dirichlet hydraulic head conditions along the lateral boundaries of the model. The discretization used in the model was chosen to provide an acceptable degree of accuracy at a reasonable computational cost.

The groundwater model included a total of 19 hydrostratigraphic and structural units that were defined based on the hydrostratigraphic framework model of Sims, et al. (1999). Each cell in the finite difference grid of the simulation domain was mapped to a specific hydrostratigraphic unit or structural material type based on its location in the hydrostratigraphic framework model. Winterle (2003, Table 2-1) lists the hydraulic conductivity values used to calibrate the model assuming steady-state conditions. This list is reproduced in Table 2-1 of this report.

Table 2-1. Material Types and Assigned Model Properties (modified from Winterle, 2003, Table 2-1)*

Material Type	Description	Hydraulic Conductivity (m/day)†	Porosity
PZ	Deep Paleozoic aquifer system	0.05	0.01
UVA	Uppermost volcanic aquifer	0.5	0.001
UVC	Upper volcanic confining unit	0.15	0.1
LVA	Lower volcanic aquifer	0.15	0.001
LVC	Lower volcanic confining unit	0.0002	0.1
Alluv (Alluvium)‡	Valley-fill alluvium	3.0	0.1
FMW (FMW_flt)‡	Fortymile Wash fault zone	5.0	0.001
BR–PBC (BR–PBC_zone)‡	Bow Ridge–Paintbrush Canyon fault zone	4.0	0.001
Cald-pz (Caldera_PZ)‡	Caldera zone: altered paleozoic rocks	0.001	0.01
Cald-vr (Caldera_VR)‡	Caldera zone: altered volcanic rocks	0.0003	0.01
SC–IR (SC–IR_flt)‡	Solitario Canyon–Iron Ridge fault zone	0.0005	0.01
SC–West (SC–West_flt)‡	Western splay of Solitario Canyon fault zone	0.0005	0.01
CF (CF_flt)‡	Crater Flat fault zone	5.0×10^{-5}	0.01
VH1 (VH1_flt)‡	VH–1 fault zone	5.0×10^{-5}	0.01
BM (BM_flt)	Bare Mountain fault zone	0.05	0.01
H95	Highway 95 fault zone	0.005	0.01
Grav1 (Grav1_flt)‡	Gravity fault zone #1	0.001	0.01
Grav2 (Grav2_flt)‡	Gravity fault zone #2	0.05	0.01
CA (CA_flt)‡	Central Amargosa fault zone	0.5	0.01

*Winterle, J. “Evaluation of Alternative Concepts for Saturated Zone Flow: Effects of Recharge and Water Table Rise on Flow Paths and Travel Times at Yucca Mountain.” San Antonio, Texas: CNWRA. 2003.
†1 m = 3.28 ft
‡The terms in parentheses appear in the legend of Figure 2-1.

The calibrated groundwater model developed in Winterle (2003) reproduced observed hydraulic heads at the site with an acceptable degree of accuracy. The mean absolute error for the 70 observation points included in the model was 9.6 m [31 ft], and the root-mean-square error was 17.3 m [57 ft]. Winterle (2003) noted that the computed root-mean-square error was less than that associated with the root-mean-square error of 30 m [98 ft] reported by the

U.S. Department of Energy (DOE) for its calibrated saturated zone site-scale model. Winterle (2003) further noted that calibration errors were smallest in the area hydraulically downgradient from Yucca Mountain. These results, therefore, build confidence in the ability of the model to simulate flow at the site-scale and, in particular, to support solute transport away from the proposed repository footprint. An order of magnitude for the porosity of each material type in the model was also presented in Winterle (2003, Table 2-1). As noted by Winterle (2003), considerable uncertainty exists with regard to the effective porosity of the material types included in the model. Uncertainty in the effective porosity for the various hydrostratigraphic units at Yucca Mountain is also included in the DOE TSPA-LA parameter set (Bechtel SAIC Company, LLC, 2004). The porosities for the materials listed in Table 2-1 do not affect the calibration of the steady-state groundwater flow model. The porosities are important, however, for determining groundwater velocities that are needed to simulate solute transport. Solute transport simulations based solely on advective displacements of particles were reported in Winterle (2003).

Advective transport scenarios performed for the Yucca Mountain region in Winterle (2003) using an earlier repository footprint produced plume dimensions (width and thickness) at the regulatory compliance boundary that were on the order of a few hundred meters. These results are informative as they provide lower bounds for the expected plume dimensions at the regulatory compliance boundary; however, they provide little information on the likely sizes of plumes and associated peak concentrations at the regulatory compliance boundary. A better understanding of the evolution of potential solute plumes from the repository footprint requires a more robust approach that includes the effects of macrodispersion and chemical diffusion. These processes result in lateral spreading of solute plumes, thereby increasing their cross-sectional area and reducing their peak concentration.

2.3 Development of a Saturated Zone Transport Model for Yucca Mountain

The model analyses in this report consider transport of a conservative nonreactive solute and represent an initial step in better understanding the effects of dispersion and source region on plume geometry and evolution. Insights gained from this work will be used to develop a more comprehensive model to simulate radionuclide transport at the site. The analyses presented in this work are also expected to provide insights related to plume geometries and potential dilution factors that will be useful for reviewing the DOE license application for the potential high-level waste repository at Yucca Mountain.

The transport model is based on MT3DMS Version 4.5 (Zheng and Wang, 1999). The code is capable of simulating advection, hydrodynamic dispersion, and diffusion of solutes in groundwater systems. Because MT3DMS does not simulate groundwater flow, it may be coupled to a groundwater flow code such as MODFLOW. For the purposes of this work, the groundwater flow model developed for the Yucca Mountain region by Winterle (2005, 2003) is used as the basis for the flow fields used in MT3DMS. Of the four scenarios evaluated in Winterle (2003), Case 2 was described as being the most representative of present-day conditions at the site. As a result, this model was selected as the flow model to support the solute transport simulations. Pre and postprocessing of MT3DMS data are performed in GMS Version 5.1 (Environmental Modeling Research Laboratory, 2005), thereby making it easy to integrate the MODFLOW output with the MT3DMS input.

2.3.1 Overview of MT3DMS Version 4.5

MT3DMS Version 4.5 is a widely used modular three-dimensional code capable of simulating advection, dispersion, diffusion, source/sink mixing, and some chemical reactions of solutes in groundwater systems. Examples of chemical reactions included in MT3DMS are equilibrium-controlled linear and non-linear sorption and first-order irreversible and reversible kinetic sorption. The code simulates solute transport using several mathematical approaches for solving the advection dispersion equation, including a traditional finite difference formulation, particle-tracking-based Eulerian-Lagrangian formulations, and a higher-order finite-volume total variation diminishing formulation. The particle-tracking-based Eulerian-Lagrangian methods in MT3DMS Version 4.5 are the Method of Characteristics, the Modified Method of Characteristics, and the Hybrid Method of Characteristics, which is a combination of Method of Characteristics and Modified Method of Characteristics. The Hybrid Method of Characteristics approach draws on the complementary strengths of the Modified Method of Characteristics and the Method of Characteristics schemes thereby mitigating their individual weaknesses. The various mathematical formulations included in MT3DMS Version 4.5 for solving the advection dispersion equation can be used with any block-centered finite difference flow model (e.g., MODFLOW). In applications with MODFLOW it is assumed that the fluid density is constant and the medium is fully saturated.

MT3DMS Version 4.5 includes a dual-domain formulation for modeling solute transport. In this approach, two distinct domains are conceptualized: a mobile domain in which advective flow occurs and an immobile domain in which diffusive transport occurs. This formulation is applicable to modeling advective transport in fractured media with diffusion of solutes into a relatively stagnant rock matrix. The dual-domain formulation requires two porosities for each finite difference grid cell: one for the mobile region and the other for the immobile region. In addition, a mass transfer coefficient is required to exchange mass between the two domains.

2.3.2 Application of MT3DMS to Simulate Saturated Zone Solute Transport at Yucca Mountain

The Hybrid Method of Characteristics transport algorithm contained in MT3DMS Version 4.5 (Zheng and Wang, 1999) was used to simulate solute transport because of its documented numerical stability, accuracy, and computational efficiency. The flow and transport simulations use similar finite difference grids, with the only difference being that only the portion of the flow simulation domain through which transport was expected to take place was used for the transport calculations. The use of the smaller domain resulted in a greater than 50-percent reduction in transport simulation times when compared to the use of the full flow model domain. The computational domains used to simulate groundwater flow and solute transport in the Yucca Mountain region are shown in Figure 2-2.

Radionuclides are expected to enter the saturated zone as a mass flux. This mass flux is included in the DOE saturated zone transport model abstraction (Bechtel SAIC Company, LLC, 2004) and is used in the convolution integral that combines it with the radionuclide breakthrough curves computed by the saturated zone transport abstraction model in an effort to simulate the mass flux entering the accessible environment. A mass flux entering the saturated zone can be represented in MT3DMS using either a mixed boundary condition (Robbins boundary condition) or a Neuman boundary condition. These boundary conditions inevitably result in a near constant concentration in water table cells after a period of time if there is no net accumulation of mass in water table cells. For the purposes of this work, a constant concentration was applied to water table cells within the repository footprint. The use of a constant concentration for these cells is reasonable given that (i) the differences in solute concentrations in evolving plumes, based on a flux-based boundary condition and an appropriately selected constant-concentration boundary conditions, are expected to be small compared to the solute concentration uncertainties caused by the hydrogeologic structure and the variable transport properties; and (ii) this work is focused on an analysis of relative concentrations rather than absolute concentrations.

Simulation grid cells along the water table that lie within the repository footprint are shown in Figure 2-3. Each simulation grid cell along the water table that lies within the repository footprint can be assigned a unique concentration with unique turn-on and turn-off times. For the purposes of this work, cells in which concentration sources were present and active were kept at constant concentration throughout the duration of the simulation [i.e., $c\ (x, y, z, t = 0) = 0$ and $c\ (x, y, z, t>0) = constant$, where c represents the solute concentration; $x, y,$ and z represent spatial coordinates; and t represents time]. The application of constant concentrations to the 300 × 300-m [984 × 984-ft] grid cells includes an implicit assumption that solutes are uniformly dispersed throughout the source cell.

Because dispersive spreading within the unsaturated zone was not considered, the maximum size of the potential source region may be underestimated. This potential underestimation may occur because dispersive spreading in the unsaturated zone can cause solutes to spread beyond the boundaries of the repository footprint. This spreading is not currently accounted for in this analysis, but may be accounted for in subsequent work by including sources in the cells that are adjacent to the repository footprint. Note that lateral flows associated with perched water zones in the region between the repository and the saturated zone may also result in radionuclide mass entering the saturated zone outside the repository footprint.

Advection and hydrodynamic dispersion were assumed to be the primary physical processes controlling plume evolution in the model. Simulations included in this report considered longitudinal dispersivity values that are consistent with those included in Bechtel SAIC Company, LLC (2004) and the TPA Version 5.0.1 code. Molecular diffusion is not currently included in the model, as its effects are assumed to be small compared to hydrodynamic dispersion during the 10,000-year simulation period considered in this report. Diffusion coefficients for the volcanics included in Bechtel SAIC Company, LLC (2004) are between 5×10^{-10} and 5×10^{-12} m^2/s [5.3×10^{-9} and 5.3×10^{-11} ft^2/s]. In addition, the dual-domain formulation present in MT3DMS Version 4.5 (Zheng and Wang, 1999) that can be used to model transport in fractured or extremely heterogeneous porous media is not included in the present work. The importance of this process will be evaluated in future transport analyses.

Porosities used in the transport simulations were identical to those used by Winterle (2003) to support the calculation of probable transport times between the repository and the regulatory compliance boundary south of Yucca Mountain. The porosities assigned to the hydrostratigraphic units in Winterle (2003) are within the respective distribution ranges for the alluvium valley-fill and volcanic units listed in Bechtel SAIC Company, LLC, (2004, Table 6-8).

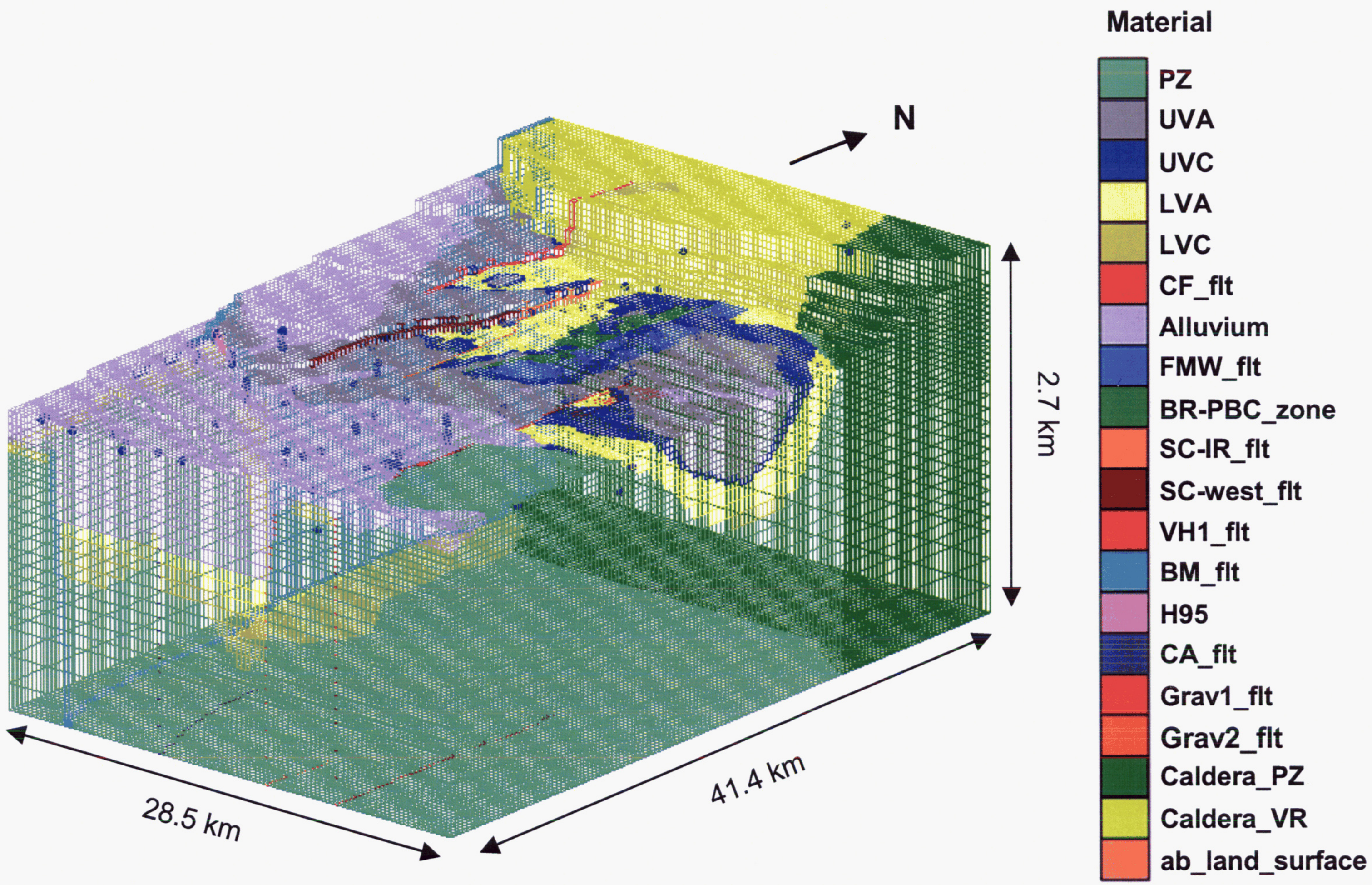

Figure 2-1. Three-Dimensional Oblique View of the Groundwater Model Domain (Including Hydrostratigraphy) Used in Winterle, et al. (2002) and Winterle (2003). The View Looks to the Northwest. [1 km = 0.62 mi]

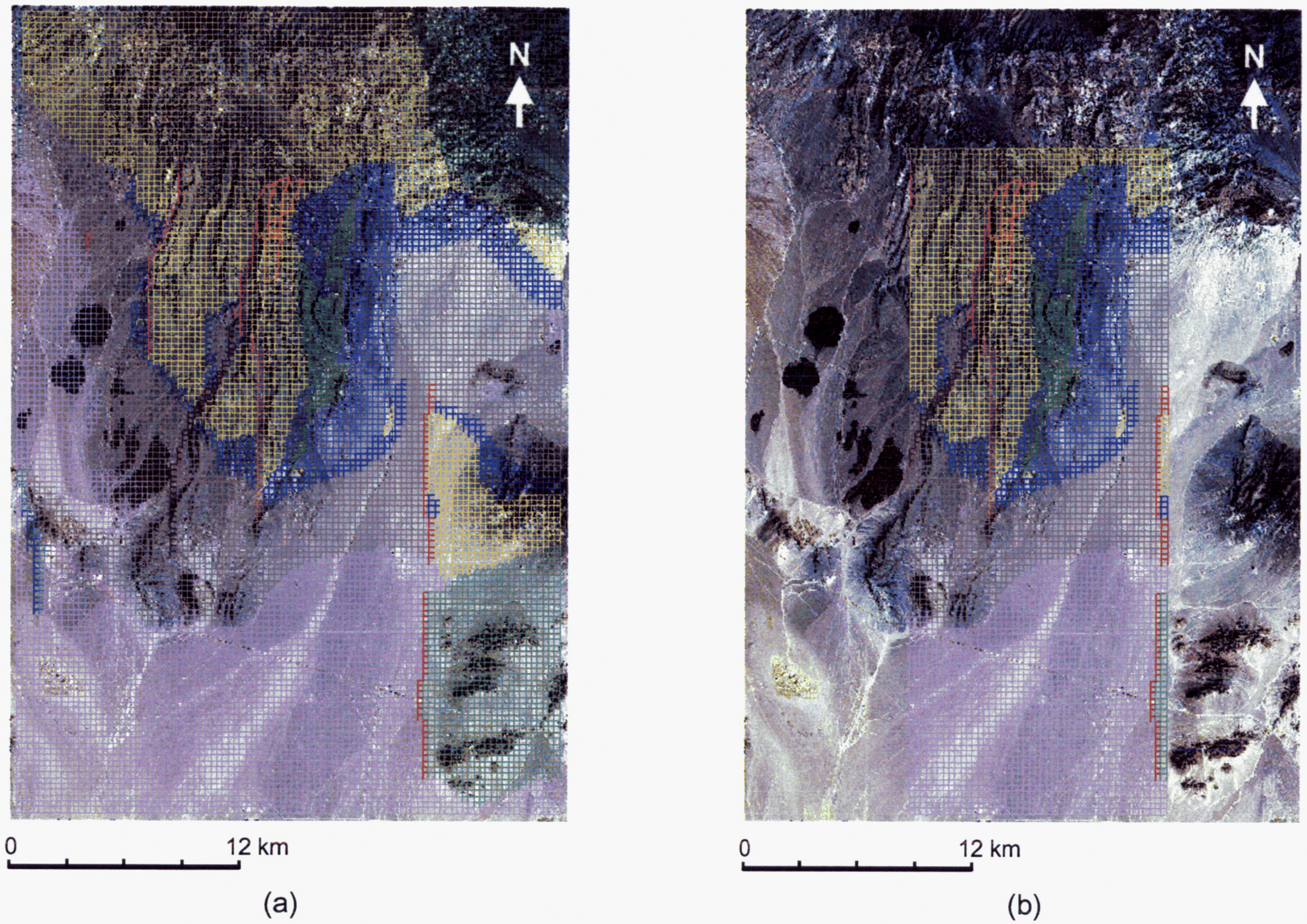

Figure 2-2. Comparison of the Simulation Grids Used for the Groundwater Flow Model and the Solute Transport Model (a) Flow Model Domain and (b) Transport Model Domain. [1 km = 0.62 mi]

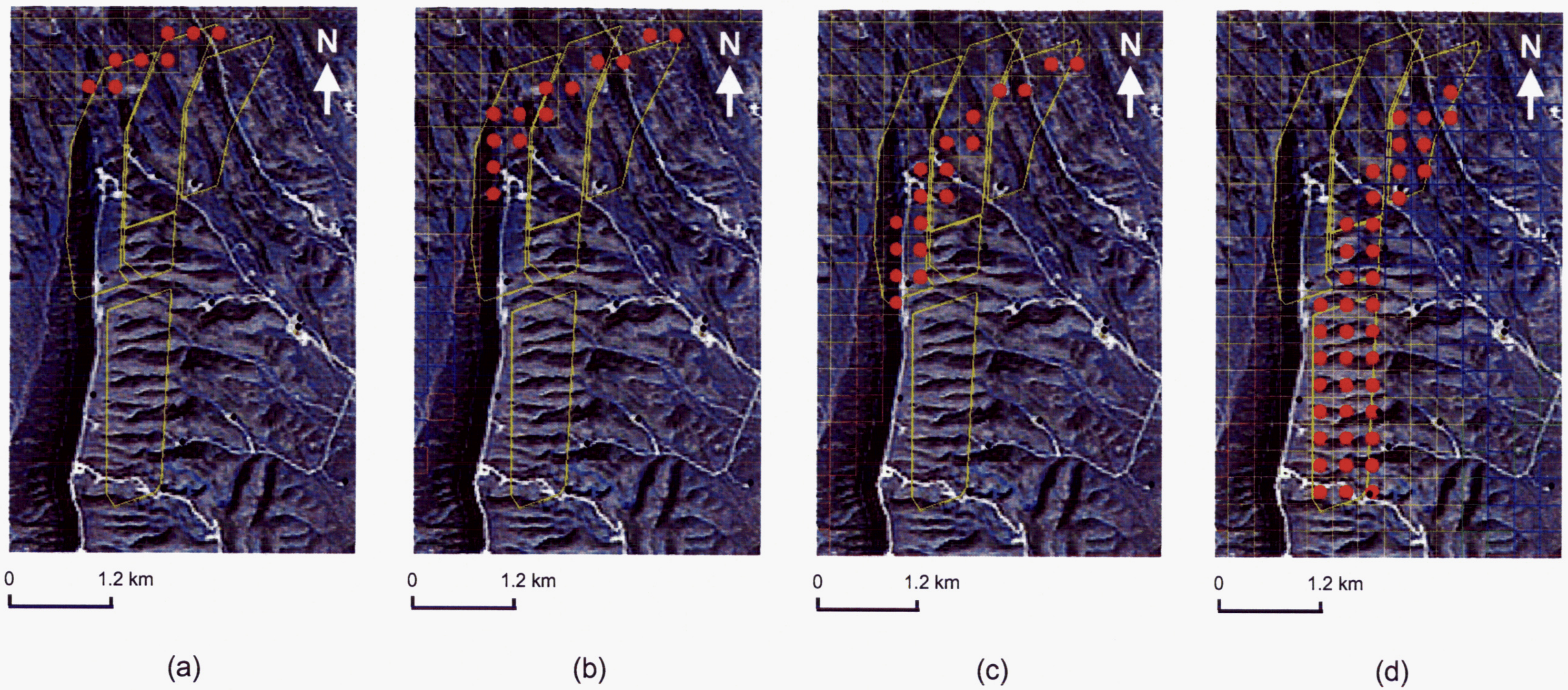

Figure 2-3. Computational Grid Cells Within the Repository Footprint (Red Dots) That May Be Used as Concentration Source Cells in the Solute Transport Simulations (a) Source Cells in Layer 3, (b) Source Cells in Layer 4, (c) Source Cells in Layer 5, and (d) Source Cells in Layer 6. [1 km = 0.62 mi]

3 SIMULATION RESULTS AND ANALYSES

3.1 Introduction

The solute transport model discussed in Section 2 was used to evaluate potential plume evolution from the repository footprint to the regulatory compliance boundary for several source and parameter scenarios. The simulations were performed for a period of 10,000 years. Each simulation required approximately 24 CPU hours on a computer with an Intel Pentium 4 3.2-GHz (512 MB-RAM) CPU.

Scenarios considered in this report focused on different potential source locations within the repository footprint. In addition, the simulations considered a range of longitudinal dispersivities and a range of ratios describing the relation of longitudinal dispersivity to horizontal and vertical transverse dispersivity. The ranges of values selected for the analysis are consistent with those used in industry, the TPA Version 5.0.1 code, and the U.S. Department of Energy (DOE) in Bechtel SAIC Company, LLC (2004). Previous analyses using the TPA code assumed the longitudinal dispersivity for the tuff volcanic units to be approximately 1 percent of the transport distance in the tuff unit, which in turn is sampled from a uniform distribution with an upper value of 17 km [10.6 mi] and a lower value of 12 km [7.5 mi]. Hence, the longitudinal dispersivity for the tuff unit used in the TPA code was between 120 and 170 m [394 and 558 ft]. The TPA code further assumed that the longitudinal dispersivity for the alluvial valley-fill was 10 percent of the transport distance in the alluvium, which varies between 1 and 6 km [0.6 and 3.7 mi] depending on the sampled transport distance in the tuff. The longitudinal dispersivity in the alluvium was therefore between 100 and 600 m [328 and 1,969 ft]. Transverse dispersivity is not accounted for in the TPA code because transport in the saturated zone was modeled using a one-dimensional stream tube.

Bechtel SAIC Company, LLC (2004) assigned identical values to the longitudinal dispersivity of the tuff and alluvium units. The assigned longitudinal dispersivities were sampled from a truncated log-normal distribution with a mean of 2.0 and a standard deviation of 0.75. This corresponds to a mean longitudinal dispersivity of 100 m [328 ft] with an upper 95-percent confidence limit of 3.2 km [2 mi]. However, as noted by DOE, the actual value of longitudinal dispersivity used in the saturated zone transport abstraction model that will be likely used to support the DOE TSPA-LA abstraction simulations is 10 percent of the sampled value (Bechtel SAIC Company, LLC, 2004). As a result, the mean longitudinal dispersivity used in the simulations is 10 m [33 ft], and the upper 95-percent confidence limit is approximately 316 m [1,037 ft]. The horizontal and vertical transverse dispersivities used in the DOE transport abstraction model are scaled to 0.5 and 0.005 percent of the longitudinal dispersivity, respectively. These ratios of transverse dispersivities to longitudinal dispersivity are small, and as a result, it is expected that solute plumes based on these ratios will be narrow and have high center-line concentrations. Dispersivity ratios commonly used by practicing environmental scientists assume the horizontal transverse dispersivity to be 10 percent of the longitudinal dispersivity and the vertical transverse dispersivity to be 1 percent of the longitudinal dispersivity (Zheng and Wang, 1999). Plumes based on these ratios are expected to demonstrate greater spreading and lower center-line concentrations when compared to those generated based on the DOE ratios. It should be noted that apart from the near 1:10 ratio between asymptotic longitudinal macro-dispersivity and asymptotic horizontal transverse macro-dispersivity computed by Freyberg (1986) for the Borden tracer experiment, lower ratios have generally been observed at other field sites. For example, field-based asymptotic macro-dispersivities reported for the Cape Cod tracer experiment by Rehfeldt and Gelhar (1992) indicate that the ratio of asymptotic longitudinal macro-dispersivity to asymptotic horizontal transverse macro-dispersivity is 1:50. For the Borden site, the enhanced transverse spreading of the tracer plume was assumed to reflect the effects of large seasonal lateral flow transients at the site. Rehfeldt and Gelhar (1992) have also argued that the magnitude of the asymptotic macro-dispersivity observed at Cape Cod may also be influenced by seasonal flow transients at the site. Strong flow lateral transients along the expected transport pathway from the repository footprint have not been reported.

The various simulations discussed in this section of the report examine the characteristics of solute plumes that may evolve in the saturated zone at Yucca Mountain based on (i) source characteristics, including size and location; and (ii) dispersivity values representative of those used in the TPA Version 5.0.1 code, the DOE transport abstraction model, and other commonly used values. The various transport scenarios considered are listed in Table 3-1.

The following sections of the report summarize the results of the three scenarios outlined in Table 3-1.

Note that the figures described in this section of the report are located at the end of this section.

3.2 Scenario 1

Scenario 1 provides insights into the range of cross-sectional dimension solute plumes migrating from Yucca Mountain that may achieve at the regulatory compliance boundary during the 10,000-year period. This scenario assumes (i) identical longitudinal dispersivity values for the tuff and alluvium hydrostratigraphic units (consistent with the DOE model) and (ii) longitudinal dispersivity values that fall within the range listed in Bechtel SAIC Company, LLC (2004).

All potential source grid cells in the transport model (i.e., all water table grid cells within the repository footprint) were active during the 10,000-year simulation period. This approach was expected to produce wide plumes that provide insights into the maximum sizes of plumes and peak concentrations that may occur at the regulatory compliance boundary as a function of dispersivity. To support the analysis, a range of longitudinal, horizontal transverse, and vertical transverse dispersivity values were used (see Table 3-1, Scenario 1). As noted in Section 2, dispersive spreading in the unsaturated zone leading to potential source sizes larger than the repository footprint was not considered. Hence, the largest plume sizes at the regulatory compliance boundary that are contained in this report may underestimate the largest solute plumes that may occur at the regulatory compliance boundary. However, the uncertainty in the horizontal transverse dispersivity values considered in the analysis may generate enough lateral spreading to compensate for the potentially smaller source region. Additionally, the scale of potential lateral spreading in the unsaturated zone is small compared to the size of the repository footprint.

For each simulation, a prescribed concentration of 10 mg/L was applied to each grid cell in the source region. For each of the four longitudinal dispersivity values considered in the scenario, two simulations were performed: one based on more commonly used ratios of longitudinal dispersivity to transverse dispersivity and the other based on the DOE ratios of longitudinal

Table 3-1. Transport Scenario Analyses

Scenario	Description
1	Objective: Determine the size of plumes that may cross the regulatory compliance boundary for selected values of longitudinal dispersivity sampled from the distribution in Bechtel SAIC Company, LLC (2004)*. Source model: All potential source grid cells within the repository footprint are active. Range of model considerations: • 10 mg/L constant concentration applied to all source cells • Longitudinal dispersivity, α_L = 300, 100, 10, and 1 m [984, 328, 33, and 3 ft] — Commonly used transverse dispersivity ratios – Horizontal transverse dispersivity (α_{TH}) ratio: $(\alpha_L/\alpha_{TH}) = 10$ – Vertical transverse dispersivity (α_{TV}) ratio: $(\alpha_L/\alpha_{TV}) = 100$ — Bechtel SAIC Company, LLC (2004)* transverse dispersivity ratios – Horizontal transverse dispersivity (α_{TH}) ratio: $(\alpha_L/\alpha_{TH}) = 200$ – Vertical transverse dispersivity (α_{TV}) ratio: $(\alpha_L/\alpha_{TV}) = 20,000$
2	Objectives: (i) Determine whether small, widely spaced plumes can cross the regulatory compliance boundary. (ii) Evaluate potentially small plumes that may cross the regulatory compliance boundary. Source models: (i) A single source grid cell in the western portion of the repository footprint is made active. (ii) Two source cells, one located in the northern portion of the repository and the other located in the southern portion of the repository. (iii) Two source cells, one located in the eastern portion of the repository and the other located in the western portion of the repository. Range of model considerations: • 10 mg/L constant concentration applied to all source cells • Longitudinal dispersivity, α_L = 100, 10, and 1 m [328, 33, and 3 ft] — Commonly used transverse dispersivity ratios horizontal transverse dispersivity (α_{TH}) ratio: $(\alpha_L/\alpha_{TH}) = 10$ – Vertical transverse dispersivity (α_{TV}) ratio: $(\alpha_L/\alpha_{TV}) = 100$ — Bechtel SAIC Company, LLC (2004)* transverse dispersivity ratios – Horizontal transverse dispersivity (α_{TH}) ratio: $(\alpha_L/\alpha_{TH}) = 200$ – Vertical transverse dispersivity (α_{TV}) ratio: $(\alpha_L/\alpha_{TV}) = 20,000$
3	Objective: Examine plume geometries at the regulatory compliance boundary that may result from using longitudinal dispersivity values sampled from the TPA Version 5.0.1 code.† Source model: All potential source grid cells in the repository footprint projected to the saturated zone are active. Range of model considerations: • 10 mg/L constant concentration applied to all source cells • Longitudinal dispersivity values (i) tuff units, α_l = 135 m [443 ft] and alluvium, α_L = 450 m [1,465 ft] and (ii) tuff units, α_L = 170 m [558 ft] and alluvium, α_L = 100 m [328 ft] — Commonly used transverse dispersivity ratios – Horizontal transverse dispersivity (α_{TH}) ratio: $(\alpha_L/\alpha_{TH}) = 10$ – Vertical transverse dispersivity (α_{TV}) ratio: $(\alpha_L/\alpha_{TV}) = 100$ — Bechtel SAIC Company, LLC (2004)* transverse dispersivity ratios – Horizontal transverse dispersivity (α_{TH}) ratio: $(\alpha_L/\alpha_{TH}) = 200$ – Vertical transverse dispersivity (α_{TV}) ratio: $(\alpha_L/\alpha_{TV}) = 20,000$

*Bechtel SAIC Company, LLC. "Saturated Zone Flow and Transport Model Abstraction." Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2004.

†The TPA Version 5.0.1 code software validation has not been completed. The use of parameter ranges from the code, therefore, represent current unofficial best estimates that may change in the official release of the code.

dispersivity to transverse dispersivity (both horizontal and vertical). The results from these eight simulations are discussed in the following paragraphs.

Figure 3-1 (a through h) shows the simulated plumes after 10,000 years in plan view at an elevation of 725 m [2,879 ft]. The figures show that the plumes initially migrate in an easterly direction before taking a more southerly path through the tuff. This migration pathway is consistent with that described by Winterle (2003) and is assumed to be influenced by the presence of the Bow Ridge–Paintbrush Canyon fault zone (Winterle, 2003). It should also be noted that the plumes presented in Figure 3-1 (a through h) are wider than the advective particle tracks presented in Winterle (2003, Figure 3-7), which were based on an identical flow field. The increased width reflects the result of including hydrodynamic dispersion.

Comparisons of the plume sizes based on the more commonly used dispersivity ratios (Figure 3-1a,c,e,g) to those based on the DOE dispersivity ratios (Figure 3-1b,d,f,h) show that the latter generally result in narrower plumes with higher center-line concentrations when compared to the former. This result is expected based on the smaller dispersivity ratios used by DOE. Comparisons of Figure 3-1a,c,e,g show that as the longitudinal dispersivity decreases and the resulting horizontal and vertical transverse dispersivity values decrease, the plumes become narrower. The simulation results also show that a significant portion of the path length of each plume is in the volcanic tuff units with the transition of the plume from the volcanic tuff units to the alluvial valley-fill occurring in the southern portion of Fortymile Wash. At the water table, the distance from the compliance boundary to the region where the plumes transition from the tuff to the alluvial valley-fill is between 3.3 and 5.2 km [2.1 and 3.2 mi]. It is expected that the reported range in the distance from the transition zone to the regulatory compliance boundary will increase as the values for the longitudinal dispersivity used in the scenario increase. Because the interface between the tuff and alluvial valley-fill dips to the south, the 5.2-km [3.2-mi] distance from the transition zone to the regulatory compliance boundary at the water table represents an effective upper bound for the travel distance in the alluvial valley-fill.

Figure 3-2a,b shows longitudinal profiles through the plumes simulated using a longitudinal dispersivity of 10 m [33 ft]. Note that a longitudinal dispersivity of 10 m [33 ft] represents the mean value used in the DOE Saturated Zone Flow and Transport Model Abstraction (Bechtel SAIC Company, LLC, 2004). The figures show the more traditional dispersivity ratios produce more vertical dispersion than the DOE ratios. For example, the region of high concentration computed using the DOE ratios occupies a narrower zone than that computed using commonly used dispersivity ratios. However, the simulation results generally show that the volcanic confining layer slows the vertical spreading of the plumes (Figure 3-2a,b).

The cross-sectional dimensions of the plumes at the regulatory compliance boundary were also measured as part of the analysis. Figure 3-3 (a through h) shows vertical sections though the eight simulated plumes at the approximate location of the regulatory compliance boundary and Table 3-2 summarizes their respective width and thickness. The figures further demonstrate that the upper and lower volcanic confining units (UVC and LVC in Figure 2-1) reduce the rate at which the plume spreads vertically. The reduced rate of vertical spreading of the plume through the volcanic confining unit is caused by the low groundwater velocity in the unit. The plume dimensions listed in Table 3-2 show that the plumes based on the more commonly used dispersivity ratios are generally wider than those based on the DOE dispersivity ratios. For example, for the case where the longitudinal dispersivity is assumed to be 300 m [984 ft], the maximum width of the plume is approximately 4.7 km [2.9 mi] for the more commonly used

Table 3-2. Summary of Simulation Results for Scenario 1*				
Longitudinal Dispersivity (m)†	Horizontal Transverse Dispersivity (m)†	Vertical Transverse Dispersivity (m)†	Maximum Plume Width (m)†	Maximum Plume Thickness (m)†
300	30	3	4,650	1,150
300	1.5	0.015	2,400	900
100	10	1	3,150	940
100	0.5	0.005	2,250	860
10	1	0.1	2,200	875
10	0.05	0.0005	2,000	810
1	0.1	0.01	1,800	750
1	0.005	0.00005	1,800	750

* Shaded rows represent data based on simulations conducted using the DOE ratios.
†1 m = 3.28 ft

dispersivity ratios and 2.25 km [1.4 mi] for the DOE dispersivity ratios. Note that, as the longitudinal dispersivity decreases, the plume dimensions converge, indicating that the advective transport is becoming the dominant process controlling the cross-sectional geometry of the plume. Figure 3-3 (a through h) shows that the plumes based on the DOE dispersivity ratios generally have higher center-line concentrations than those based on the more commonly used dispersivity ratios.

In addition to estimating the dimensions of the eight plumes simulated in Scenario 1, the annual groundwater flow through the plumes at the location of the regulatory compliance boundary was also estimated. This estimation was performed in the Groundwater Modeling System environment using the cell-based water budget calculation option. The annual groundwater flow through the eight plumes at the location of the regulatory compliance boundary is between 0.67×10^6 and 1.74×10^6 m^3/yr [545 and 1,410 acre-ft/yr] where the lower annual groundwater flow corresponds to a longitudinal dispersivity of 1 m [3 ft] and is similar for both the commonly used dispersivity ratios and the DOE dispersivity ratios. The larger annual groundwater flow corresponds to the model in which the longitudinal dispersivity of 300 m [984 ft] was used in conjunction with the commonly used dispersivity ratios. For the plume based on the DOE dispersivity ratios and a longitudinal dispersivity of 300 m [984 ft], the annual groundwater flow through the plume at the location of the regulatory compliance boundary was 0.92×10^6 m^3/yr [750 acre-ft/yr]. This flow represents an upper value for the simulations based on the DOE dispersivity ratios that were considered in this report.

3.3 Scenario 2

Scenario 2 provides insights into whether independent widely spaced small sources can produce distinct plumes that cross the regulatory compliance boundary without significant commingling. It is currently assumed that a single consolidated plume will cross the regulatory compliance boundary. Scenario 2 examines this assumption. In addition, the simulations performed under Scenario 2 provide a means to evaluate potentially small plumes that may migrate from the repository footprint.

To support this investigation, several numerical simulations were performed using small localized sources. Some simulations included a single small localized source placed at a fixed location within the repository footprint. These simulations provided information on the evolution of small solute plumes from the repository footprint and are useful for examining plume dilution factors. Other simulations performed under this scenario examined whether solute plumes emanating from small localized sources in the northern and southern portions would evolve as separate plumes or whether they would merge into a single plume along the transport pathway. A similar analysis was also conducted using localized sources located in the eastern and western sections of the repository footprint. The various simulations considered in Scenario 2 are summarized in Table 3-1.

3.3.1 Can Multiple Independent Plumes Cross the Regulatory Compliance Boundary?

Simulation results for the case in which localized small sources were placed in the northern and southern portions of the repository show that initially the plumes evolved separately with both plumes migrating toward the southeast before turning toward the south (Figure 3-4a,b). The general location of the transition from an easterly migration path to a more southerly path is consistent with that observed in Scenario 1. South of the repository footprint, the migration paths of the two plumes appear to converge (Figure 3-4a,b). This convergence is caused in part by convergent groundwater flows south of the repository location that are associated with the Bow Ridge/Paintbrush fault systems. Plumes from simulations involving sources located in the eastern and western portions of the repository also converged (Figure 3-5a,b). However, when compared to the simulations involving sources located in the northern and southern portions of the repository, convergence occurred much closer to the repository footprint. This occurred because the sources in the eastern and western portions of the repository footprint were located along flow lines that were in close proximity. The convergence of the plume migration paths south of the repository therefore suggests that it is unlikely that for the given flow model conceptualization, independent widely spaced plumes will cross the regulatory compliance boundary.

Table 3-3 summarizes the dimensions of the various plumes at the location of the regulatory compliance boundary, and Figure 3-6a,b provides cross sections through the plumes in Figure 3-5a,b. As expected, the plume dimensions listed in Table 3-3 are smaller than those listed in Table 3-2 when similar dispersivity values are compared. Furthermore, plumes based on the more commonly used dispersivity ratios produced plumes that were as wide as or wider than those based on the DOE dispersivity ratios. Table 3-3 shows that the lateral dimensions of the plumes associated with the northern and southern sources are larger than those associated with the eastern and western sources. The enhanced spreading associated with the simulations involving northern and southern sources relative to those involving eastern and western sources may indicate that there is still a small separation between the center lines of the plumes associated with the northern and southern sources.

Table 3-3. Summary of Simulation Results for Scenario 2: Dual Source Models*					
	Longitudinal Dispersivity (m)†	Horizontal Transverse Dispersivity (m)†	Vertical Transverse Dispersivity (m)†	Maximum Plume Width (m)†	Maximum Plume Thickness (m)†
North and South Sources	100	10	1	2,200	800
	100	0.5	0.005	1,800	500
	10	1	0.1	1,700	500
	10	0.05	0.0005	1,700	460
	1	0.1	0.01	1,500	450
	1	0.005	0.00005	1,500	450
East and West Sources	100	10	1	1,800	675
	100	0.5	0.005	1,350	525
	10	1	0.1	1,075	500
	10	0.05	0.0005	1,150	480
	1	0.1	0.01	900	450
	1	0.005	0.00005	900	450

* Shaded rows represent data based on simulations conducted using the U.S. Department of Energy ratios.
†1 m = 3.28 ft

3.3.2 Evolution of Small Plumes Within the Saturated Zone

The potential characteristics of small plumes migrating through the saturated zone south of the repository footprint were analyzed as part of Scenario 2. The concentration source used for this analysis was the western source in Figure 3-5a,b. Longitudinal dispersivity values used to support the analysis are summarized in Table 3-1.

Figure 3-7a,b shows examples of the various plumes produced by this simulation. Plumes simulated under this scenario are qualitatively consistent with those simulated in Scenario 1 as they show that the dispersivity ratios used by DOE produce narrower plumes at the regulatory compliance boundary after 10,000 years when compared to plumes computed based on more commonly used dispersivity ratios. Table 3-4 shows that, for each longitudinal dispersivity value considered, plumes based on the DOE and commonly used dispersivity ratios are marginally different. However, as shown in Figure 3-8a,b, noticeable differences are observed when the cross-sectional areas of the various plumes are compared. These differences result in differences in the annual groundwater flow through the plumes. The groundwater flow through the simulated plumes is between 0.2×10^6 and 0.4×10^6 m^3/yr [170 and 320 acre-ft/yr], with the upper value reflecting the case in which a longitudinal dispersivity of 100 m [328 ft] is used with the commonly used dispersivity ratios and the lower value reflecting the cases in which a longitudinal dispersivity of 1 m [3 ft] is used with both the commonly used dispersivity ratios and the DOE dispersivity ratios.

Table 3-4. Summary of Simulation Results for Scenario 2: Single Source Models*				
Longitudinal Dispersivity (m)†	**Horizontal Transverse Dispersivity (m)†**	**Vertical Transverse Dispersivity (m)†**	**Maximum Plume Width (m)†**	**Maximum Plume Thickness (m)†**
100	10	1	1,350	525
100	0.5	0.005	1,200	525
10	1	0.1	1,000	450
10	0.05	0.0005	1,000	450
1	0.1	0.01	900	425
1	0.005	0.00005	900	425

* Shaded rows represent data based on simulations conducted using the U.S. Department of Energy ratios.
†1 m = 3.28 ft

Effective dilution factors were also computed for each plume at the regulatory compliance boundary. For the purposes of this analysis, the effective dilution factor was computed by dividing the cross-sectional area of the plume at the regulatory compliance boundary by the cross-sectional area of the source cell. The computed dilution factors for the simulated plumes were between 20 and 34. The higher dilution factor reflects the case in which the commonly used dispersivity ratios were used with a longitudinal dispersivity of 100 m [328 ft], and the lower value reflects the case in which the DOE dispersivity ratios were used with a longitudinal dispersivity of 1 m [3 ft].

3.4 Scenario 3

Scenarios 1 and 2 assume a common longitudinal dispersivity for the tuff and alluvium hydrostratigraphic units. Recent analyses using the TPA Version 5.0.1 code, however, assigned different longitudinal dispersivity values to the tuff and alluvium hydrostratigraphic units. The range of longitudinal dispersivity values sampled in the TPA code for both the tuff and allivium hydrostratigraphic units is in the upper range of those listed in Bechtel SAIC Company, LLC (2004). Scenario 3 is similar to Scenario 1 with two exceptions: (i) separate longitudinal dispersivity values were assigned to the tuff and alluvium hydrostratigraphic units and (ii) longitudinal dispersivity values used in the simulations were exclusively within the range used in the TPA code.

Two base models were considered in this scenario. In the first model, the plume travel distance in the tuff hydrostratigraphic unit was assumed to be 13.5 km [8.4 mi]. This distance is within the range observed in Scenario 1 for the travel distance within the tuff units at the water table. Based on this travel distance, the TPA Version 5.0.1 code would assign a longitudinal dispersivity of 135 m [443 ft] to the tuff hydrostratigraphic units and a longitudinal dispersivity of 450 m [1,476 ft] to the alluvium hydrostratigraphy. In the second base model, the plume travel distance in the tuff hydrostratigraphic unit was assumed to be 17 km [10.6 mi]. This travel distance is somewhat consistent with transport pathways deeper in the tuff aquifer system.

For this model, the TPA code would predict longitudinal dispersivity values of 170 and 100 m [557 and 328 ft] for the tuff and alluvium hydrostratigraphic units, respectively. All potential source cells within the repository footprint were made active for each model.

The simulation results presented in Figure 3-9a,b and Figure 3-10a,d show that longitudinal dispersivities in the range of values computed by the TPA Version 5.0.1 code are capable of producing rather wide plumes at the location of the regulatory compliance boundary after 10,000 years. Table 3-5 summarizes the various plume geometries produced by the simulations. In particular, the simulation results show that as the travel distance in the tuff increases, the plume dimensions at the compliance boundary decreases due to the decrease in the longitudinal dispersivity in the alluvium. In addition, the results show that the smallest plume produced by assuming the DOE dispersivity ratios has a width on the order of 2 km [1.2 mi]. Longitudinal cross sections through the plume produced by the first model using the commonly used dispersivity ratios show that in some local areas the plume appears to penetrate the Paleozoic units. Computed annual groundwater flow rates through the plumes at the regulatory compliance boundary are between 0.83×10^6 and 1.23×10^6 m^3/yr [671 and 1,000 acre-ft/yr].

Table 3-5. Summary of Simulation Results for Scenario 3*

Longitudinal Dispersivity (m)†	Horizontal Transverse Dispersivity (m)†	Vertical Transverse Dispersivity (m)†	Maximum Plume Width (m)†	Maximum Plume Thickness (m)†
Alluvium = 100 Tuff = 170	Alluvium = 10 Tuff = 17	Alluvium = 1 Tuff = 1.7	3,300	1,025
Alluvium = 100 Tuff = 170	Alluvium = 0.5 Tuff = 0.85	Alluvium = 0.005 Tuff = 0.0085	2,000	900
Alluvium = 450 Tuff = 135	Alluvium = 45 Tuff = 13.5	Alluvium = 4.5 Tuff = 1.35	4,500	940
Alluvium = 450 Tuff = 135	Alluvium = 2.25 Tuff = 0.675	Alluvium = 0.0225 Tuff = 0.00678	2,400	900

* Shaded rows represent data based on simulations conducted using the U.S. Department of Energy ratios.
†1 m = 3.28 ft