3-D Model Validation in Support of Site Closure, Material Disposal Area L, Los Alamos, NM - 11545

Philip H. Stauffer*, Kay H. Birdsell*, and William J. Rice**

*Mail Stop T-003, Los Alamos National Laboratory, Los Alamos NM, 87545 ** Mail Stop T-991, Los Alamos National Laboratory, Los Alamos NM, 87545

ABSTRACT

An updated three-dimensional numerical model of a volatile organic compound (VOC) vapor plume in the subsurface at Los Alamos National Laboratory is developed using a site-scale numerical model. The site-scale numerical model evolved over many years (1999–2006) and has been used to evaluate the nature and extent of the subsurface contaminant 1,1,1-trichloroethane (TCA) associated with waste disposal. This model was next refined to include a 2006 soil-vapor extraction (SVE) pilot test and calibrated permeabilities for the site were developed to match flow-rate versus pressure drop and concentrations in the exhaust gas. Here, we present results of a blind validation simulation that begins with the pre-SVE test in 2006 and predicts present day (2010) plume concentrations. The data/model correlation coefficient (r²) for over 150 data model pairs is greater than 90% in the year 2010. The ability of the model to align with data after four years that include two active SVE demonstration tests provides confidence that the model captures the dominant physical transport processes at this site, and can thus be used with confidence to explore future scenarios of site behavior. We next present calculations of long-term transport to the regional aquifer under different conditions of uncertainty, and show that uncertainty in the effective diffusion coefficient in the 100-m thick Cerros del Rio basalt that directly overlies the regional aquifer has a large impact on uncertainty in predicted mass flux to the aquifer. Finally, we present results that show how potential SVE performed in the years 2011-2013 could affect system behavior, reducing long-term impacts at the regional aquifer. Results from the validated model are currently being used to determine if SVE is an appropriate remedial action for this site.

INTRODUCTION

Material Disposal Area L (MDA L) is located within Los Alamos National Laboratory (LANL) on the narrow finger mesa, Mesita del Buey, on the Pajarito Plateau to the southeast of the town of Los Alamos, NM, approximately 5 km from the Rio Grande. This liquid waste disposal facility received VOC waste from 1975 to 1985, with the waste emplaced in shafts reaching to depths of 18 m (60 ft.). The upper 91 m (300 ft) of the site is composed of the Bandelier Tuff, underlain by rocks of the Cerros del Rio Basalt flows. The geology of the site is discussed in more detail in Stauffer et al., 2005 and references therein [1]. The modeling presented in this work is used to predict potential future impacts that the VOC plume may have on ground water to support decisions on remedial alternatives that may be undertaken during site closure.

Numerical simulations are used to determine the subsurface transport of VOCs from MDA L. The simulations presented build on many years of work performed to use site data in numerical models to better understand the nature and extent of VOC contamination at MDA L [1-7]. Specifically, calculations are presented using the numerical models developed to explore more scenarios related to the corrective measures evaluation (CME) and the possible role of SVE at MDA L [6-7]. Previous analysis showed that SVE has the potential to effectively remove significant quantities of VOCs from the subsurface [5]. Suggestions regarding sampling frequency and location were made based on these results to allow for rapid detection of any sudden changes in the plume [6]. Estimates of the radii of influence of the SVE pilot test wells (~ 37 m (120 ft)) were given, and a suggestion was made that two SVE wells be installed to remove VOC mass near the bottom of the plume [6]. Figure 1 shows an aerial photograph of MDA L, with the site boundary outlined in black. Two distinct groups of waste bearing shafts are responsible for the observed TCA plume.

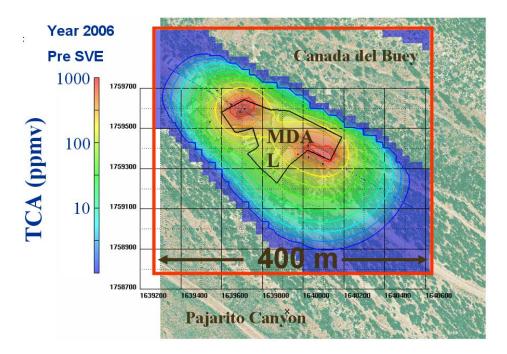


Fig. 1. Concentration contours of TCA on a plane 24 m (80 ft) bgs in 2006 before the SVE pilot test. This modeled plume serves as the starting point for the blind validation to 2010 data.

MODEL DISCUSSION

Table 1 lists physical properties relevant for TCA transport. The dimensionless Henry's Law coefficient (H ($(\text{mol}_{TCA}/L_{air})$ / $(\text{mol}_{TCA}/L_{water})$)) has been corrected for temperature using the Van't Hoff equation [8]. The dimensionless coefficient used in the modeling (H = 0.458) corresponds to a temperature of 15°C, which is the average between the average surface temperature at MDA L (approximately 10°C) and the water table at a depth of 1000 ft (20°C). For all calculations of concentration just above the water table, the simulated vapor concentration times H = 0.57 = C_g/C_1 (subscripts refer to gas and liquid) is used to calculate groundwater concentrations at 20°C. Supporting site data for porosities and permeabilities can be found in Tables II and III of [4] and [6].

Table I Physical properties of TCA (modified from [1]).

Parameter	Value		
Molecular weight	133 g/mol		
Liquid density	1325 kg/m³ (at 293 K)		
Vapor pressure	100 mmHg (at 293 K)		
Water solubility (mg/L)	950 mg/L (at 293 K)		
Tuff sorption coefficient K _d	< 0.08 mL/kg fully saturated		
Henry's Law constant (H _{TCA})	62 MPa/(liquid mole fraction) equal to 0.458 (g/L) _{vapor} /(g/L) _{liquid} (at 288.5 K)		
Diffusion coefficient in crushed Bandelier tuff assumed to be nearly equal to that of TCE. From Trujillo et al., 1998 [9]. $J = -\theta_a D$ gradC	4.6e-6 to 9.3e-6 m ² /s at 2%–7% relative saturation		
where J is flux, θ_a is volumetric air content, C is the vapor concentration, and D is the diffusion coefficient.	4.4e-7 to 1.4e-6 m ² /s at 29%–36% relative saturation		

Two shaft fields at MDA L, one on the east and one on the west, generate VOC vapors that diffuse away from the shafts to create a subsurface vapor plume. These two source regions can be seen on Figure 1. VOCs in liquid waste or in pore water volatilize to form soil vapor as determined by Henry's Law partitioning. It is likely that the previous vapor concentrations were higher than current levels because uncontainerized wastes would evaporate and enter the subsurface more readily than containerized wastes. This effect would be more prevalent at the eastern shaft field because those shafts were used first and disposal operations (e.g., containerization) improved with time. Under natural conditions, the shape and growth of the plume are diffusion driven [1]. Vapor-phase diffusion is a relatively rapid process that is faster than unsaturated liquid flow at MDA L and accounts for the observed migration to depth of VOCs in soil vapor within the Bandelier Tuff [1]. Diffusive growth is somewhat buffered by Henry's Law partitioning; as the vapor plume migrates, it partitions into uncontaminated pore water, which acts as a sink for VOCs and, in turn, slows the diffusive process. Diffusion theoretically spreads contamination spherically along concentration gradients. However, topography plays an important role in vapor transport at MDA L. The atmosphere operates as a zero concentration boundary along the top and sides of the mesa, causing the steepest concentration gradients to be toward the surface. This leads to preferential vapor transport toward the external mesa boundaries vielding releases to the atmosphere, as observed from a surface flux survey conducted at the site [9]. Asphalt, which currently covers the site, decreases this mechanism somewhat because it blocks the vapors from exiting at the surface [1]. Diffusive gradients also spread soil vapors downward toward the regional aquifer. Shallow vapors will tend to diffuse out of the mesa at the surface while deeper vapors may diffuse downward. Uniform diffusive behavior is thought to occur in the high porosity Bandelier Tuff [1].

It is uncertain if diffusion through the low-porosity fractured Cerros del Rio basalt will be dominated by molecular processes or if possible barometric influences could lead to higher effective diffusion in these rocks. Open, interconnected air pathways probably occur between the top of the Cerros del Rio volcanic series and the regional aquifer beneath MDA L. Lithologic logs for well R-54, located 305 m (1000 ft.) west of MDA L, indicate that 113 m (372 ft) of Cerros del Rio volcanics overlie 24 m (80 ft) of basaltic sediments in the vadose zone near MDA L. The Cerros del Rio sequence is a stratified stack of massive lava flows separated by interflow breccias, cinder and scoria beds, and volcanic sediments. This volcanic sequence is made up of approximately 50% lavas and 50% porous interflow deposits. Lava flows (generally < 6 m (20 ft) thick) are separated by interflow breccias and thick deposits of porous cinder and scoria. Borehole video logs indicate the lavas are variably fractured. Air pathways in these volcanic rocks include high- and low-angle fractures in the massive lava flows and open interconnected pores in the breccias, cinders, scoria, and sediments. The basaltic sediments beneath the Cerros del Rio rocks consist of porous sands and gravels. Previous work has shown that the basalt is likely connected to outcrops within 3-4 km [10], allowing the basalt to be in equilibrium with atmospheric pressure. One possible effect of this connectivity on TCA transport would be to increase the apparent diffusion coefficient within the basalt [11]. Although poorly constrained by data, we fix the basalt porosity to 10% for all simulations presented, thus taking a conservative approach that will lead to high estimates of mass flux to the regional. Because we are solving a diffusion problem, diffusive flux is directly proportional to the porosity, and reduction in porosity from 10% to 1% will lead to a reduction in diffusive flux by a factor of 10. Previous work performed to simulate a vadose zone infiltration experiment suggests that the actual effective porosity of the basalt is much lower than 10% [12]. However these results are based on liquid water flow, and we cannot rule out the possibility that the vapor phase will see a larger effective porosity.

During active SVE, advective air flow dominates vapor-phase migration. Vacuum applied during extraction pulls air containing vapors to the extraction borehole. During the SVE test, vapors were extracted near the two higher-concentration areas near the shaft fields. This removal of higher concentration vapors can slow subsequent diffusion away from the source areas or even reverse gradients toward the extraction boreholes following SVE [6].

MODEL FORMULATION

The porous flow simulator Finite Element Heat- and Mass-Transfer (FEHM) is used for all calculations [13,14]. Briefly, the simulations account for the growth of a vapor-phase TCA plume under various site conditions. Three temporal stages of simulation lead to the model results. The first two stages were originally conducted earlier and recreated to form the basis for the current study [1,4-7]. In order to judge the quality of the model throughout the modeling process, spatially-dependent, TCA concentration data from the site and the predicted (modeled) concentrations are compared through linear regression.

The first stage simulates waste emplacement and plume growth through 2006 [1,4]: These modeling studies were used to determine the primary drivers for the growth of the plume from 1975-2006 and to confirm that our conceptual model could recreate the measured site data. The models account for diffusive plume growth from the shaft fields according to the timing of original waste emplacement (e.g., the eastern shafts were filled before the western shafts), and follows plume growth through time starting in 1975 and ending in 2006 before the start of the SVE pilot test[1]. Higher concentrations near the shaft fields (up to 15,000 parts per million by volume (ppmv) near the eastern shaft fields and 6000 ppmv near the western shaft field) are used initially to represent potential uncontainerized leaks (1975-1983), which match early monitoring data. These source concentrations are decreased in time (down to 1000 and 2000 ppmv at the east and west sources, respectively) to match site data, and the upper boundary condition was modified at the appropriate time (1985) to account for the addition of asphalt pavement [1]. Diffusion coefficients in the Bandelier Tuff were calibrated during this modeling phase (Table II). No advective transport of TCA due to flow of pore water or subsurface air is included in the initial diffusion model, and therefore, the numerical solution did not require the input of rock permeability values. Henry's Law partitioning is included to represent the interaction of the TCA in the vapor plume with pore water. Figure 1 shows a slice through the modeled plume in the year 2006 on a plane 24 m (80 ft.) below the surface.

Table II Porosity, Saturation, and Effective Diffusion Coefficient Values Used in the Simulations

Unit	Effective Porosity	In-Situ Saturation	D* (m²/s)
Qbt 2	0.41 ^a	0.06 ^b	3 x 10 ⁻⁶
Qbt 1vu	0.49 ^a	0.15 ^b	2 x 10 ⁻⁶
Qbt 1vc	0.49 ^a	0.15 ^b	2 x 10 ⁻⁶
Qbt 1g	0.46 ^a	0.15 ^b	2 x 10 ⁻⁶
Cerro Toledo (Qct or CT)	0.45 ^a	0.40	5 x 10 ⁻⁷
Otowi Member (Qbo)	0.44 ^a	0.35	5 x 10 ⁻⁷
Cerros del Rio basalt (base case diffusion)	0.1 ^b	0.02	3 x 10 ⁻⁶
Cerros del Rio basalt (2x free-air diffusion)	0.1 ^b	0.02	1.56 x 10 ⁻⁵
Land surface	0.48 ^c	0.02	3 x 10 ⁻⁶
Asphalt	0.5 ^c	0.02	1 x 10 ⁻¹⁴
Shafts	0.5°	0.02	3 x 10 ⁻⁶
Wellbore	1.0	0.001	3 x 10 ⁻⁶
Well Casing	0.5	0.001	1 x 10 ⁻¹⁴

The second stage simulates an SVE pilot test conducted at the site in 2006: This model starts with the model input parameters and the TCA concentration distribution in 2006 developed in the first phase and then imposes the

conditions of the SVE test to drive flow toward the extraction holes [4-7]. The numerical grid was updated to add the 2 extraction boreholes used in the test. The model was calibrated to data gathered during the SVE test (applied vacuum, extraction rate, and TCA extraction concentration as functions of time) to generate permeability distributions (Table III) that fit the data [7]. Whereas the diffusion model discussed above did not consider air movement and did not require permeability distributions, modeling of SVE requires these to properly model vapor migration during active extraction. This modeling stage also looked at hypothetical plume growth under differing scenarios, including significant increases in the source term and longer-term effects of SVE [4].

The third stage of the simulations is the current study, a blind validation of the model: The current study starts with the model setup and parameters determined during the first two modeling stages and the calibrated plume distribution before the 2006 SVE pilot test to predict forward to current conditions and beyond. We simulate four years of plume evolution during both the SVE pilot test and the subsequent diffusive plume growth to the year 2010 and compare model results to recent data. In addition, future plume growth is predicted based on scenarios that include 3 yrs of SVE, asphalt removal, and uncertainty in the diffusive behavior of the Cerros del Rio basalt. These scenarios are discussed below.

Table III Calibrated Permeabilities in both the Horizontal and Vertical Directions Used for the SVE Pilot Test Simulations

	SVE West Permeability m ²		SVE East Permeability m ²	
Unit	х,у	z	х,у	Z
Qbt 2	7.66E-13	5.41E-13	6.01E-13	9.63E-13
Qbt 1vu	7.07E-12	2.36E-12	9.83E-13	1.60E-13
Qbt 1vc	1.20E-13	6.74E-13	1.29E-11	1.97E-12
Qbt 1g	1.18E-13	6.05E-13	1.97E-13	4.87E-12
Qtt (TT)	5.90E-13	5.90E-13	6.44E-13	6.44E-13
Qct (CT)	5.90E-13	5.90E-13	6.44E-13	6.44E-13
Qbo	1.77E-13	1.77E-13	1.93E-13	1.93E-13

Note: Results are from AMALGAM calibration [7].

As described in [4], a novel wellbore mesh approach that embeds a two-dimensional (2-D) radial wellbore solution into a three-dimensional (3-D) mesh is used in the model to accurately capture the applied vacuum in the vapor extraction wells. This algorithm was recently improved to better represent the coupling term between the 2-D wellbore and the 3-D mesh. This difference in the FEHM formulation required recalibration of the estimates of permeability in the Bandelier Tuff to again match the SVE pilot test data

The 3-D simulation domain is described in detail in [4,7]. Boundary and initial conditions are discussed in detail in [4] and [7]. These same boundary conditions were used for the simulations presented here, and additional boundary conditions are also explored. The bottom boundary in the initial modeling was fixed to no-flow because this boundary was considered to be far from the evolving plume. However, the long-term simulations of the current analysis require that we explore how the bottom boundary affects concentration at the base of the vadose zone and mass transfer to the regional aquifer. For this reason, we examine both a no-flow bottom boundary and a fixed zero-concentration bottom boundary. The first leads to the highest concentrations at the base of the vadose zone while the second leads to the highest concentration gradients to depth and subsequently yields the highest estimates of flux to the regional aquifer.

The long-term water-phase infiltration rate to the regional at MDA L is thought to be on the order of 0.001 to 0.01 m/yr, and because this flux is not expected to impact the simulation results, unsaturated water flow is not included in the simulations presented. Also, the effects of naturally occurring air flow from barometric pressure or temperature changes at the surface and within the vadose zone are not included, as these effects are also expected to be small given the low topographic relief and small depth over which significant barometric effects occur [11,15,16].

The data-model regression for the starting point of the current round of simulations is quite good for the time period of 1975-2006 (pre-SVE pilot test) with an r² correlation coefficient of greater than 0.89. The model overestimates the vapor concentration at depths greater than approximately 250 ft below ground surface (bgs), but only by a few parts per million. The goal of the 2006 pre-SVE calibration is not to match every point in space exactly but to have a model that captures a large percentage of the concentration data and the overall behavior of the vapor plume without spatial and temporal bias. This exercise gives confidence that the initial conditions for the 3-D SVE simulations are good representations of the actual plume beneath MDA L in 2006. Figure 1 shows a horizontal slice of TCA concentrations in the vapor phase for the initial state (pre-SVE pilot test), and the two source areas located at the east and west shaft fields are evident in the figure. Table II contains all porosity, saturation, and diffusion coefficients used in the modeling. The recalibrated permeabilities used for the SVE Pilot Test matching and future SVE scenarios are included in Table III.

BLIND MODEL VALIDATION

The pre-2006 SVE simulations were next run to the year 2010 to test the ability of the model to predict the future under both active SVE and diffusion dominated conditions. By comparing with TCA concentration data collected during late 2009 and early 2010 pore-gas monitoring the model results can be checked to determine whether the model predictions honor the spatial and temporal development of the TCA plume approximately 4 yr after the start of the SVE pilot test. The concentration data are based on statistical averaging of the most recent four sampling quarters, which span the period from the third quarter of fiscal year (FY) 2009 to the second quarter of FY2010 [17]. VOC data for 156 monitoring ports in 26 pore-gas monitoring boreholes are used to generate the data set, which is a combination of field screening and analytical data sets. If a given port has analytical data, those concentrations are used. A correlation was established between field-screening data and analytical data from sampling ports that have both measurements available. The correlation was applied to field-screening locations without analytical data to form a more spatially complete data set.

The 2000–2006 component of the original diffusion simulations found that fixed concentrations of 2000 ppmv and 1000 ppmv in the west and east source regions, respectively, provided a good match to field data during that time. These fixed source concentrations were thus used from the end of the 2006 SVE pilot test to simulate the plume rebound to the year 2010. Figure 2A shows the data-model correlation for the blind calibration. The correlation is good, with an r^2 of 0.95 and a regression line close to the 1:1 data-model correlation. There are outlier points on the regression lines that the model does not fit, but the fact that a majority of the 156 monitoring points in 26 separate monitoring wells within the plume closely align suggests that the model is able to reasonably predict future plume behavior.

Figure 3 shows a vertical slice through the axis of the mesa contoured for both the data and the model. The slices are not exactly coincident; however the result confirms visually that the model and data are in good agreement. We reiterate that this model validation was truly blind; no parameters were adjusted to make the model prediction fit the 2010 data set.

Finally, to evaluate whether the shafts are still sources of contamination for the vadose zone, a simulation was run for which no source of TCA is included following the SVE test (mid-2006 until 2010) (Figure 2B). The data-model correlation for this case does not cluster around the 1:1 line as well as the simulations with the continuous sources, the model significantly under-predicts concentrations, and the r^2 is reduced to 0.74. This poorer fit indicates that the shafts are likely a continuing source of TCA vapors.

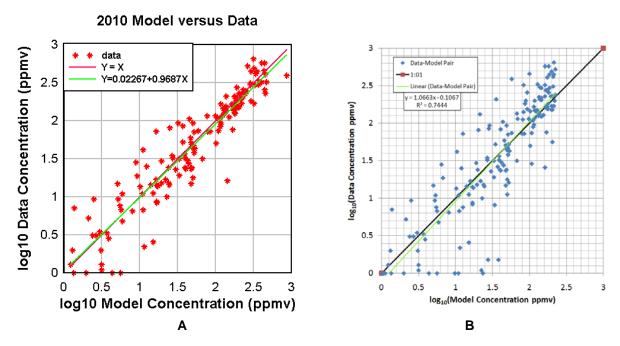


Fig. 2. 2010 Model versus data regression for A) Blind validation run from pre-2006 SVE plume through 2010 and B) same simulation but with the two source areas removed.

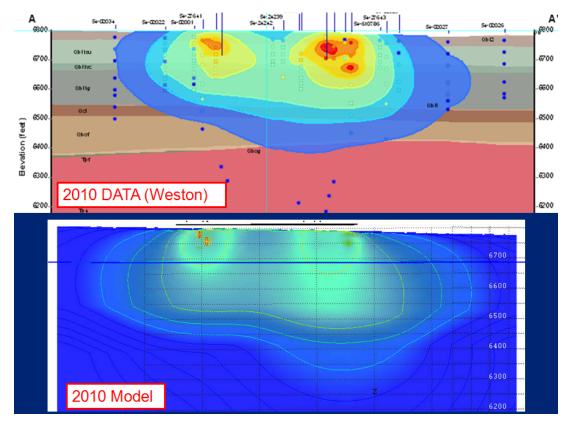


Fig. 3. Comparison of data from 2010 to the 2010 blind model validation. Although the color bars differ, the red values in both figures correspond to concentrations of approximatly 2000 ppmv.

DECISION ANALYSIS

In this section, we describe how modeling results can be used to guide decisions in selecting possible remediation alternatives. Results are first presented to examine how running the available SVE system might affect the extent of the plume in the future. For this example, the SVE system is run for 3 years, 2011-2013, and then the plume is allowed to evolve to the year 2275, 300 years in the future. To demonstrate the impacts of SVE, simulations both with and without SVE are run. Two different boundary conditions are applied to the bottom of the domain which represents the interface between the unsaturated zone and the regional water table aquifer, 1) a no-flow boundary to maximize long term concentration at the water table, and 2) a fixed zero concentration boundary to maximize mass flow to the regional aquifer. We present plots of both mass flow to the regional aquifer and concentrations of TCA in the unsaturated zone just above the regional water table. Additional uncertainty in the long term simulations is explored by including changes in the vapor-phase diffusion coefficient in the basalt meant to capture effects of increased spreading due to barometric pumping. The effect of enhanced diffusion through the Cerros del Rio basalt is simulated by increasing the base case diffusion coefficient of 3×10^{-6} m²/s to 2 times the free air diffusion coefficient of TCA $(1.56 \times 10^{-5} \text{ m}^2/\text{s})$.

SVE cycle scheme 2011 to 2013

This section describes how the hypothetical SVE interim measure is run in stages for 3 years from 2011 to 2013. The western SVE system is first run for 30 d at 2.4 m³/min (85 standard cubic feet per minute (scfm)), followed by a rest period of 30 d; then, the eastern SVE system is run for 30 d at 2.4 m³/min (85 scfm) followed by a rest of 30 d. This cycle is repeated for 3 yr. The total TCA mass (including both vapor and pore water contributions) drops from near 900 kg in 2010 to 400 kg in 2013.

Long-Term Impact near the Regional Water Table

Figure 4 shows the time-dependent calculated mass flow rate of TCA to the regional aquifer for four cases. These cases all use a zero-concentration boundary to maximize the mass flow rate to the regional aquifer. The mass flow rate is summed over the entire $410 \text{ m} \times 310 \text{ m}$ bottom boundary. The four cases explored are:

Two cases, using no SVE from 2011 to 2013 with both the base case diffusion coefficient (D*) for the Cerros del Rio basalt and the 2x free air diffusion coefficient,

Two cases with SVE from 2011 to 2013 with both the base case diffusion coefficient (D*) for the Cerros del Rio basalt and the 2x free air diffusion coefficient,

Figure 5 shows the time-dependent calculated concentration of TCA in pore water at a node that is located below the eastern source area and <u>just above</u> the water table for the same cases described above. However, these cases all use a no-flow boundary to maximize the concentration in the vadose zone above the water table. Note that the maximum contaminant level (MCL) for TCA in New Mexico is $60 \mu g/kg$. Further dilution of these predicted concentrations would occur upon mixing with the regional aquifer.

The following observations can be made:

3 yr of active SVE done in 2011-2013 can significantly impact the long-term evolution of the plume. The mass flow rate to the regional is reduced for both base case and high basalt diffusion, and concentrations at the bottom of the unsaturated zone are reduced by a significant amount.

Uncertainty in basalt diffusion leads to large changes in predicted concentrations and mass flow rates. This shows that better characterizing this parameter could reduce model uncertainty.

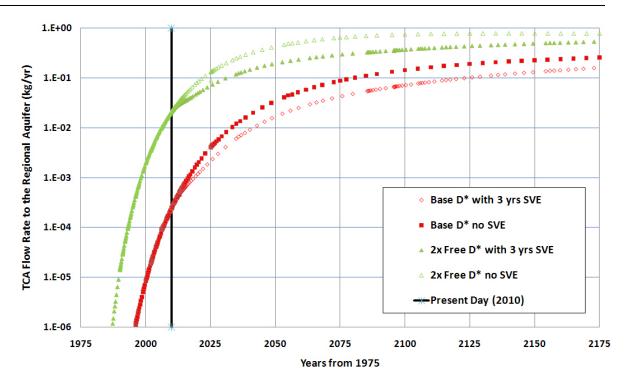


Fig. 4 TCA mass flow rate to the regional aquifer assuming a zero concentration bottom boundary. D* is the effective porous medium diffusion coefficient.

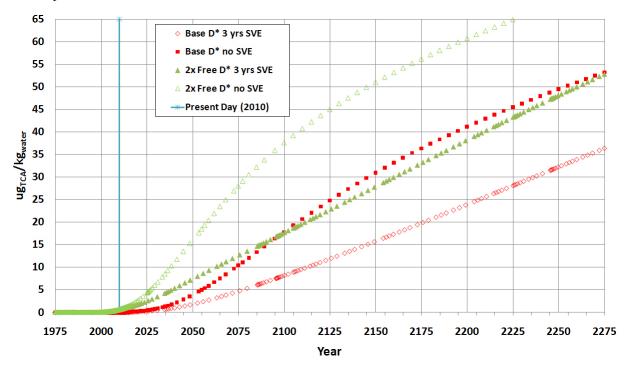


Fig. 5 TCA concentration in the pore water just above the regional aquifer assuming a no-flow bottom boundary. The MCL for TCA is $60 \mu g/L = 60 \text{ ppbm}$. D* is the effective porous medium diffusion coefficient.

In all cases, the simulations predict that concentrations will continue to increase because diffusion from the continuous source leads to continued plume growth. This prediction is based on the assumption that the source remains constant. Vapor sampling data indicate that source concentrations are declining, so this assumption is conservative. These long-term predictions for behavior of the plume near the water table are more uncertain than the shorter-term predictions in the high concentration portions of the plume near the shafts. Uncertainties are from the unknown future release of VOCs at the site, unknown diffusive characteristics of the basalt, the effect of the bottom boundary condition on flux toward the water table, and the effective porosity of the basalt.

CONCLUSIONS

This paper presents a blind model validation for TCA transport at MDA L at Los Alamos National Laboratory. The validation covers a four year period during which an active SVE pilot test was performed. The model was tested by running a blind simulation in which the assumptions and parameters were not varied, and the simulations were continued to the year 2010. TCA concentration data from 156 monitoring points in 26 separate wells were used to compare to the model results. The model plume has a 0.95 r² correlation coefficient with no evidence of spatial bias. The blind model validation provides confidence that the conceptual model and numerical implementation capture the bulk of the plume behavior under both diffusion-controlled (pre- and post-extraction) and advection-controlled (extraction) conditions.

The validated model was then used to predict the impacts of a potential SVE remedial action in the years 2011 to 2013. The models predict that 53% to 63% of the current TCA mass can be extracted over a 3-yr period based on the assumed extraction rates. In addition, SVE performed in the period of 2011 to 2013 will have a positive effect on the long-term plume behavior and could potentially significantly reduce breakthrough concentrations at the water table over the next 10 to 300 years. Much of this benefit is due to extraction of higher concentration regions of the plume that are due to former higher concentration releases. With these concentrations remediated, concentrations should not rebound to previous high values. The simulated order of magnitude of the mass removal and the spatial and temporal effects on the plume are expected to be a reasonable approximation of the general behavior of the plume under conditions similar to those used during calibration. These models can be used to provide input on other remedial alternatives, potential SVE design criteria (e.g., different extraction intervals or timing), and information on monitoring design (e.g., frequency and placement).

It is important to note that the conceptual assumption that the source can be defined as a constant-concentration source is also uncertain. Concentrations in the source region will likely decrease with time as the source diminishes; this is supported by site data.

The model results are less certain for predictions of plume migration toward the regional aquifer than for behavior near the surface. The predictions illustrate that the vapor plume will continue to diffuse downward with time and eventually may reach the regional aquifer depending on actions taken nearer the surface. Diffusion through the Cerros del Rio basalt was identified as a key uncertainty that can affect plume growth near the base of the plume. Also, the assumed bottom boundary condition used in the model affects predicted flux toward the regional aquifer. A zero-concentration lower boundary will enhance predicted plume migration toward the aquifer more than a noflow boundary. Because there is uncertainty related to plume migration toward the regional aquifer, SVE has been recommended for this site.

REFERENCES

- Stauffer, P.H., K.H. Birdsell, M.S. Witkowski, and J.K. Hopkins, Vadose Zone Transport of 1,1,1-Trichloroethane: Conceptual Model Validation through Numerical Simulation, *Vadose Zone Journal*, Vol. 4, pp. 760–773. (2005).
- 2. Neeper, D.A., Investigation of the Vadose Zone Using Barometric Pressure Cycles, *Journal of Contaminant Hydrology*, Vol. 54, pp. 59-80. (2002).
- 3. Neeper, D.A., and P. Stauffer, Unidirectional Gas Flow in Soil Porosity Resulting from Barometric Pressure Cycles, *Journal of Contaminant Hydrology*, Vol. 78, pp. 281-289. (2005)
- 4. Stauffer, P.H., J.K. Hopkins, and T. Anderson, February 25–March 1, 2007. A Soil Vapor Extraction Pilot Study in a Deep Arid Vadose Zone, Part 2: Simulations in Support of Decision Making Processes, Waste Management Conference 2007, February 25–March 1, 2007, Tucson, Arizona. (2007).
- 5. Anderson, T, P.H. Stauffer, J. Hopkins, B. Stewart, P. Mark, A Soil Vapor Extraction Pilot Study in a Deep Arid Vadose Zone, Part I: Field Study Summary, Waste Management Conference 2007, February 25–March 1, 2007, Tucson, Arizona (2007).
- Stauffer, P.H., J.K. Hopkins, T. Anderson, and J. Vrugt, July 11, 2007. Soil Vapor Extraction Pilot Test at Technical Area 54, Material Disposal Area L: Numerical Modeling in Support of Decision Analysis, Los Alamos National Laboratory document LA-UR-07-4890, Los Alamos, New Mexico. (2007).
- 7. Vrugt, J.A., P.H. Stauffer, T. Wöhling, B.A. Robinson, and V.V. Vesselinov, May 2008. Inverse Modeling of Subsurface Flow and Transport Properties: A Review with New Developments, *Vadose Zone Journal*, Vol. 7, No. 2, pp. 843–864. (2008).
- 8. EPA, http://www.epa.gov/athens/learn2model/part-two/onsite/esthenry.html accessed on Aug 21st 2010. Temperature dependence of Henrys coefficient for 1,1,1 TCA.
- 9. Trujillo, V., R. Gilkeson, M. Morgenstern, and D. Krier, June 1998. Measurement of Surface Emission Flux Rates for Volatile Organic Compounds at Technical Area 54, Los Alamos National Laboratory report LA-13329, Los Alamos, New Mexico. (1998).
- 10. Neeper, D.A., Investigation of the vadose zone using barometric pressure cycles, J. of Cont. Hydrology,(54), 59-80. (2002).
- 11. Auer, L.H., Rosenberg, N.D., Birdsell, K.H., and E.M. Whitney, The effects of barometric pumping on contaminant transport, J. Cont. Hydrology, 24(2), (1998).
- 12. Stauffer, P.H. and W. J. Stone, Surface Water\Groundwater Connection at the Los Alamos Canyon Weir Site: Part 2. Modeling of Tracer Test Results, *Vadose Zone Journal* 2005 4: 718-728.
- 13. Zyvoloski, A.G., FEHM: A control volume finite element code for simulating subsurface multi-phase multi-fluid heat and mass transfer. Los Alamos Unclassified Report LA-UR-07-3359. (2007).
- 14. http://en.wikipedia.org/wiki/FEHM; accessed on Nov 10th, 2010.
- 15. Stauffer, P.H., Auer, L.H., and Rosenberg, N.D., Compressible gas in porous media: A finite amplitude analysis of natural convection, *Int. J. of Heat and Mass Transfer*, 40 (7), 1585-1589
- 16. Stauffer P.H., and Rosenberg, N.D., Vapor phase transport at a hillside landfill, *Environmental and Engineering Geoscience*, Vol. VI, No. 1, p. 71-84.

17. LANL (Los Alamos National Laboratory), July 2010. "Periodic Monitoring Report for Vapor-Sampling Activities at Material Disposal Area L, Solid Waste Management Unit 54-006, at Technical Area 54, Second Quarter Fiscal Year 2010," Los Alamos National Laboratory document LA-UR-10-3957, Los Alamos, New Mexico. (2010).