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The SELECT Environmental Remedy Selection Tool: A Platform for T2VOC Multiphase Transport Modeling

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ABSTRACT

The SELECT project at Lawrence Berkeley Laboratory aims to develop integrated software for selecting environmental remediation strategies that maximize health-risk reduction and minimize cost. SELECT will integrate existing state-of-the-art models for site characterization, exposure, health risk assessment, remediation cost, atmospheric transport, and subsurface multiphase transport. For subsurface transport, current plans are to use the multiphase simulator T2VOC for up to three phases (aqueous-gas-NAPL) and three components (water, air, volatile organic compound) as well as heat. The prototype contaminated site currently being investigated by the SELECT project team has a thick (~30 m) vadose zone where disposal of volatile organic compounds has occurred since the early 1950's. Preliminary simulations with T2VOC show that soil vapor extraction performed with an impermeable cap in place leads to immediate reductions in soil-gas trichloroethylene concentrations under residences 200 m away from the extraction well. The simulated concentrations calculated by T2VOC will be used in the SELECT methodology to calculate exposure potential and associated carcinogenic health risk for various scenarios. The risk-cost analysis in SELECT will help managers make decisions on remediation strategies.

The effective assessment of subsurface contamination and design of appropriate and cost-effective remediation schemes requires analyses in the fields of geology, hydrology, toxicology, chemical engineering, and finance, among others. The various analyses are normally performed separately by different individuals or teams. Each of the analyses can be complex, involving approximations, uncertainties, and modeling that are likely to be current topics of research within each individual field. As such, the analyses, data collection, reporting, assessment of uncertainties, and modeling tend to be particular to each field and may not be immediately accessible or useful to the specialists in the other fields. Because of this disciplinary isolation, it is frequently difficult for the remediation manager to synthesize all of the information and results to make optimal decisions. Ir addition, there is costly duplication of effort. Taken together, these aspects of the current methodology of environmental assessment and remediation can lead to high costs and poor decision making.

With the goal of increasing the quality and lowering the costs of environmental assessment and remediation, SELECT will integrate existing state-of-the-art models for site characterization, atmospheric transport, multiphase subsurface transport, exposure, health risk assessment, and financial analyses of remediation. SELECT will run on PCs and workstations and serve as a platform from which the different components of a remediation analysis can either be performed independently or in an integrated manner. The design of SELECT emphasizes rigorous and defensible analyses within each component. As such, SELECT is designed to be used by specialists in the various component fields. The data, interpretations, and results of analyses for each component will be available in a common format for use by the other components of SELECT. The complete analysis can then be reviewed by site managers who would make decisions given the integrated analyses performed by the specialists using SELECT.

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In the case of volatile organic compounds (VOCs), subsurface contamination can lead to exposures by direct ingestion of contaminated well water or by volatilization during showering (1), or by direct entry of contaminated soil gas into the residence (2, 3, 4). When reasonable assumptions are made about factors such as the amount of water ingested and amount of time spent in the house, and spent showering, VOC concentrations in soil gas and tap water can be converted to exposures and doses by way of exposure pathway factors (5). Relating exposures over time with individual and population health risks is an important part of the SELECT methodology which will allow risk-based decision making. In addition, SELECT will compare possible hazards from contaminants to background hazards in the diet, and in the air and water, and present the uncertainties in the analysis.

In this paper, we present preliminary simulations of soil vapor extraction (SVE) of trichloroethylene (TCE) from the contaminated subsurface at McClellan Air

Force Base in Sacramento, California. We model the evolution of TCE in soil gas at the site of original contamination and at an off-base residence 200 m away during disposal and remediation. Although the T2VOC simulator is fully capable of multiphase flow simulation, we have used large grid blocks in the present analysis which prevent the formation of free phase VOC at the injection rates appropriate for the site. Thus the simulations are for single-phase soil-gas transport. We assume implicitly here that soil-gas contaminant concentrations can be related to health risks, even if these risks are very small for the present scenario. The analysis presented gives a taste of the power of integrating remediation analyses by means of subsurface flow simulation. The simulations show the transport modeling component of the SELECT methodology. The link between the selected remediation scheme and its effect on exposures at distance from the site of remediation can only be made by using a powerful and efficient transport model such as T2VOC.

MULTIPHASE SUBSURFACE TRANSPORT

Many subsurface environmental contamination problems involve infiltration of contaminated water in the vadose zone, or flow of non-aqueous phase liquids (NAPLs) above or below the water table. We have chosen the three-dimensional integral finite difference simulator T2VOC (6, 7, 8) to model these multiphase flow processes in SELECT. T2VOC is part of the TOUGH2 family of codes developed at Lawrence Berkeley Laboratory (9, 10). T2VOC models the subsurface flow and transport of three phases (aqueous, gas, and non-aqueous phase liquid [NAPL]) and three components (water, air, VOC) as well as heat. The specific VOC to be modeled is selected by specification of appropriate physical properties in the input file. Relative permeability and capillary pressure effects are also defined in the input file. While able to model the complex physical processes associated with multiphase flow in the subsurface, T2VOC retains the conceptual simplicity of the integral finite difference method (IFDM) upon which it is based. In the IFDM, there is little of the mathematical abstraction associated with other methods (e.g., the finite element method), and sparse gridding can be used for quick approximate or preliminary calculations. The user is expected to have experience in multiphase transport modeling. Even large problems with the order of 10,000 grid blocks can be run on PCs (11). One of the most powerful features of TOUGH2 is the residual formulation and fully-coupled solution technique that is capable of efficient solution of highly nonlinear flow problems (12).

CASE STUDY FOR CONTAMINANT TRANSPORT

As a case study for the development of SELECT, we are analyzing VOCs at McClellan Air Force Base in Sacramento, CA. We have chosen Operational Unit D (OU D) for its proximity to off-base residences, long history of investigation and remedial action, and because it is currently the site of remedial actions such as SVE and groundwater pump-and-treat. VOCs were disposed of into trenches and waste pits at OU D between the early 1950s and mid-1980s. TCE has been detected off-base in the subsurface west of OU D in groundwater and in soil gas (13, 14). These contamination problems have prompted remedial actions including placing off-base residents on municipal water supply, capping the waste pits, SVE, and groundwater pump-and-treat.

We report here on a preliminary numerical simulation analysis of the disposal, migration, and remediation of TCE in the vadose zone at OU D. The emphasis is on showing how SELECT will link actions and effects in space and time in the subsurface through the use of the multiphase subsurface transport model T2VOC. We model the changes in soil-gas TCE concentration below an off-base residence when disposal and remediation are performed 200 m away on-base at the site of TCE disposal. We assume that higher TCE concentrations in soil gas lead to higher exposures and greater potential health risk. However, we note that inhalation of soil gas in the residence contaminated at the levels of the present study is far less important an exposure pathway than ingestion of groundwater contaminated at levels detected in monitoring wells at the site. Thus in an actual application of SELECT, where potential exposures from groundwater and soil gas were both considered, the greatest health risks would be from ingestion of groundwater. In this case, remediation decisions would be based mostly on either cleaning up the groundwater or eliminating its use, rather than variations in the application of SVE. Although soil-gas TCE causes little health risk at the residence in the present study, the modeling of the evolution of the soil-gas plume in response to different SVE scenarios adequately illustrates the use of T2VOC for analyzing remediation scenarios in the SELECT methodology.

The scenario we consider involves 10 years of TCE disposal (beginning in 1960) followed by 20 years of natural evolution (ending in 1990). Then we simulate two remediation schemes: (1) SVE alone; and (2) SVE with an impermeable cap over the area of disposal. Both schemes effectively reduce TCE concentrations in the disposal trench itself. However, when we examine the reduction in off-base soil-gas TCE concentrations for the scenario with and without a cap, we will observe clearly that SVE with an impermeable cap in place will reduce TCE concentrations at the off-base residence immediately while SVE without a cap will not.

We present in Figure 1 a map of OU D. The oval-shaped shaded area shows the location of the soil-gas VOC plume as defined by shallow soil gas

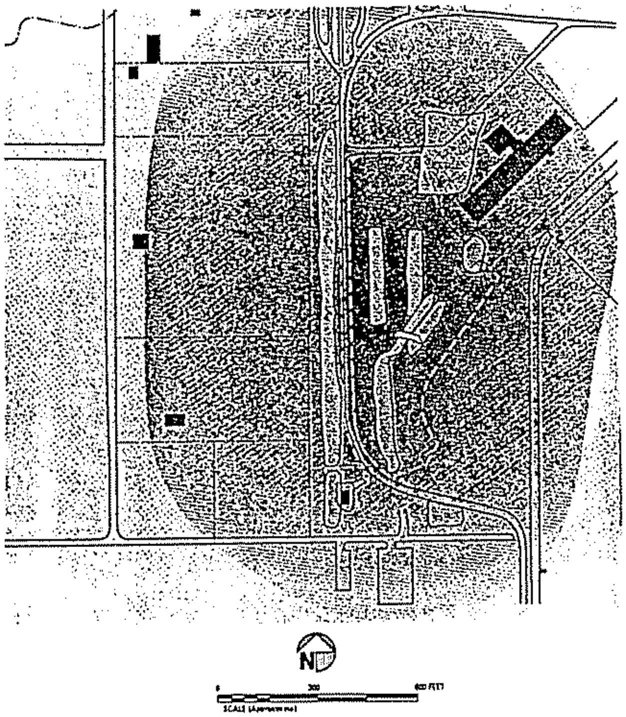

Fig. 1. Map of OU D (from 14).

measurements. The lightly shaded and irregular elongated features trending north-south and northeast-southwest are filled disposal trenches. The dark rectangular features on the west side are off-base residences. OU D is underlain by heterogeneous interbedded silt, clay, and sand (14). Porosity and permeability are highly variable, although prior gas-phase transport calculations have assumed uniform porosity and permeability (14) and we make the same assumptions here. We use intrinsic permeabilities of 5×10^{-12} m^2 in the horizontal and 1×10^{-12} m^2 in the vertical, 20 times smaller than those used in the prior study (14). The residual liquid saturation in the vadose zone is fixed at 20%, with the water table held at a constant depth of 30 m. We assume for simplicity zero infiltration due to rainfall and a constant temperature of 20 °C. Even with zero infiltration, we will see that the cap plays an important role in remediation.

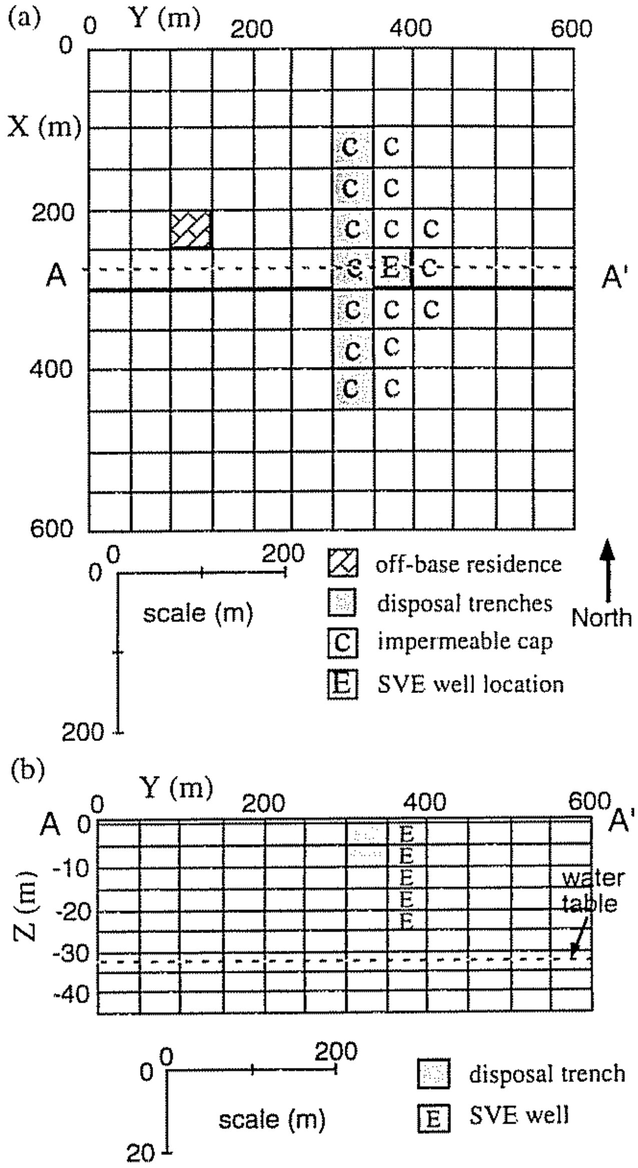

Fig. 2. (a) X-Y plane discretization for the OU D TCE disposal simulation. The off-base residence, disposal trenches, and cap location are shown. (b) Y-Z plane cross section A-A' showing the disposal trenches and water table at 30 m. Note 5x vertical exaggeration.

The three-dimensional space discretization is shown in Figure 2 in plan view and in cross section. In Figure 2a, the eight shaded grid blocks (7 aligned north-south, 1 to the east) represent the disposal trenches, the brick pattern is the off-base residence, and the C's represent locations of the cap. The cap also covers the eastern-most trench grid block which is also the site of the SVE extraction well. Grid blocks in the topmost layer (see Figure 2b) are used to model the ground surface where pressure is constant and TCE is immediately diluted by atmospheric mixing. For the modeling of the cap, the top layer of grid blocks comprising the cap are made impermeable. All other boundaries of the domain have no-flow boundary conditions.

Approximately 3.5×10^4 kg of TCE were discharged into the waste trenches over about 10 years (14). This is approximated by specifying a uniform injection of TCE at a rate of 6.9 x 10^{-6} kg/s for 10 years into each of the 16 grid blocks below the waste trenches. Because of the relatively coarse discretization, free-phase TCE does not form. That is, there is sufficient volume of gas in the pore spaces of each grid block to fully vaporize the injected TCE. With liquid saturation already at its residual saturation, we are modeling only gas-phase flow where the air and vaporized TCE components flow by diffusion and advection. While free-phase TCE was in the past present near and directly beneath the disposal trench, the approximation that TCE is entirely in the gas phase and as a dissolved component in the immobile residual aqueous phase is probably valid for longer time scales and for the majority of the domain away from the immediate vicinity of the trench. The physical properties of TCE are mostly taken from (15) and are presented along with relevant models for the various transport processes in (6, 7). Relevant parameters for the problem are presented in Table 1.

Table 1. Parameters for OU D simulation.

quantity	value	units
porosity (ϕ)	.2	–
X-, Y-permeability ($k_Y = k_X$)	5 x 10^{-12}	m^2
Z-permeability (k_Z)	1 x 10^{-12}	m^2
residual liquid saturaton	.2	–
fraction organic carbon (foc)	.003	–
ref. TCE diffusivity (d)	8 x 10^{-6}	$m^2\ s^{-1}$
tortuosity (τ)	1.	–
TCE disposal rate	6.9 x 10^{-6}	kg s^{-1}
productivity index for SVE well	2.8 x 10^{-11}	m^3

In the scenario presented here, there is a 32.5 m-thick vadose zone initially consisting of air devoid of TCE in equilibrium with residual water with a gas-static initial pressure distribution. TCE is injected into the second and third layers of grid blocks below the disposal trenches for 10 years. TCE transport is by gas-phase diffusion and by advection driven by pressure and density effects. The spread of TCE in the gas phase is shown in Figure 3 after 10 years. We observe TCE concentrations greater than 10^6 ppbv (parts per billion by volume) in the disposal trenches and rapid decline with distance away from the trench such that TCE concentration in the shallow subsurface 200 m west (at the site of the off-base residence) remains essentially zero. From t = 10–30 years, the source of TCE is turned off and the plume continues to spread by natural evolution (Figure 4). We see that TCE concentrations have spread significantly, but still decline by 4 orders of magnitude over the 200 m from the trench to the off-base residence. This decline with distance in the concentrations is consistent with results of shallow soil-gas surveys (14).

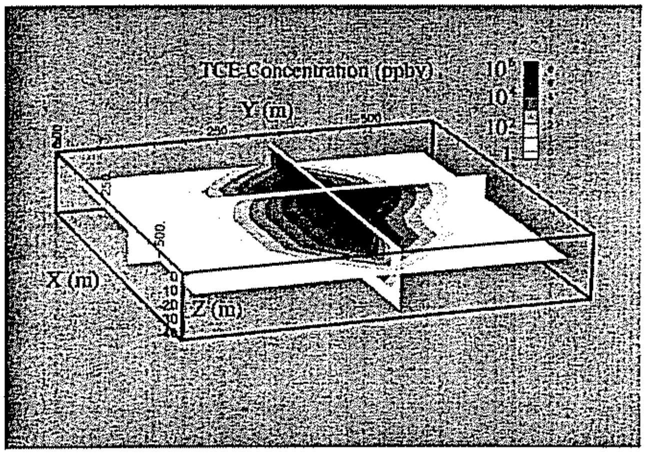

Fig. 3. Soil-gas TCE concentration (ppbv, parts per billion by volume) after 10 years of TCE disposal.

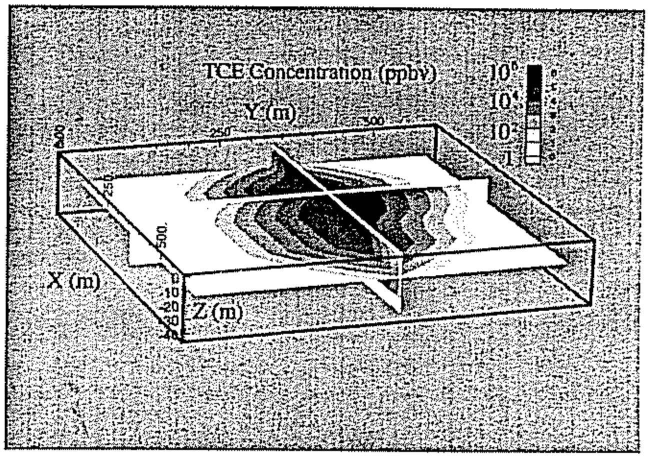

Fig. 4. Soil-gas TCE concentration (ppbv) after 20 years of natural evolution (no TCE disposal).

At t = 30 years, SVE is started under two different scenarios: (1) without a cap in place over the disposal trenches; and (2) with the cap. The SVE is modeled using the well-on-deliverability model (16, 17) where a column of grid blocks is assumed to comprise the screened well and a vacuum of 7 inches of Hg (2.37 x 10^4 Pa) (18) below atmospheric pressure is held in the extraction well. To model a narrow well bore in these large grid blocks, we use a productivity index (PI) equal to 2.8 x 10^{-11} m^3. Results at t = 40 years (after 10 years of SVE) are shown for both of these scenarios in Figures 5 and 6, respectively. Comparing Figures 5 and 4 we observe that TCE concentrations have declined in the vicinity of the disposal trench but that the total volume of contaminated soil continues to increase. Examination of Figure 6 reveals that both concentration in the

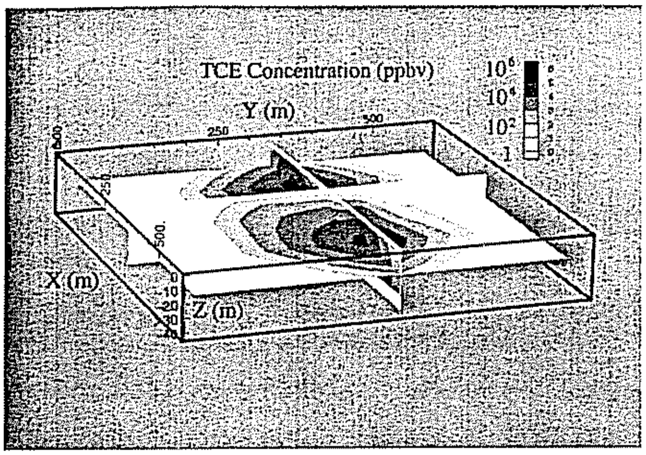

Fig. 5. Soil-gas TCE concentration (ppbv) after 10 years of SVE without a cap.

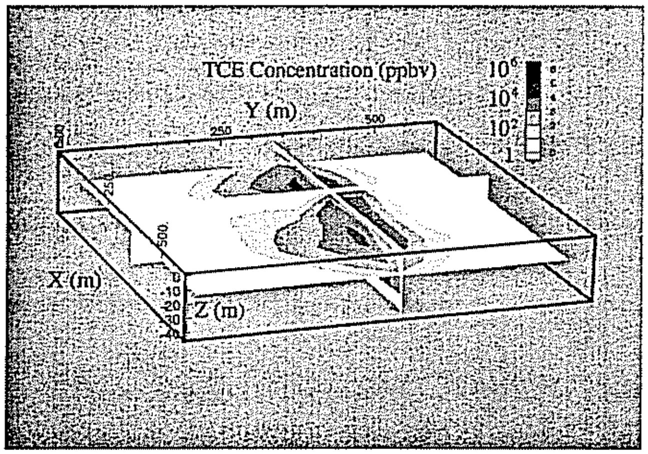

Fig. 6. Soil-gas TCE concentration (ppbv) after 10 years of SVE with a cap.

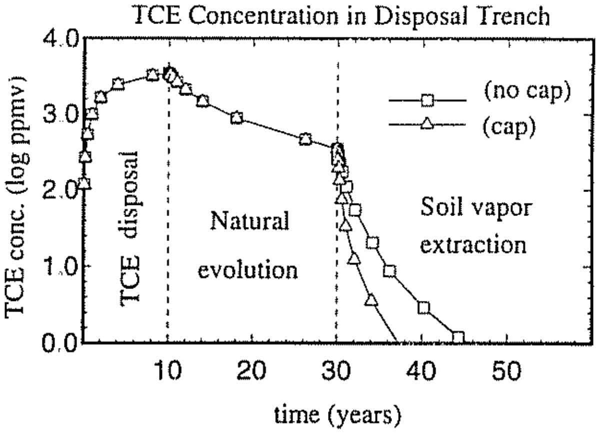

Fig. 7. Soil-gas TCE concentration (log ppmv) vs. time in the disposal trench for the cap and no-cap scenarios. The periods of application of the different actions are labeled and separated by the vertical dashed lines.

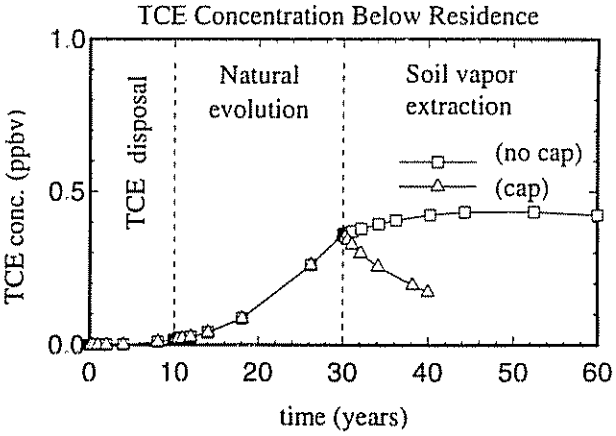

Fig. 8. Soil-gas TCE concentration (ppbv) vs. time below the residence for the cap and no-cap scenarios.

trench and the total volume of contaminant has declined when SVE is applied with a cap in place. We show in Figure 7 the evolution of TCE concentration in a grid block within the disposal trench for the two different remediation scenarios. As seen in Figures 5, 6, and 7, both the cap and no-cap schemes reduce TCE concentrations effectively in the disposal trench.

In Figure 8 we show the evolution of TCE concentration 2.5 meters below the off-base residence. A no-action scenario would result in continuing increases in TCE concentration approximately along the curve extrapolated from t = 30 years in Figure 8. SVE with and without a cap both reduce TCE concentrations relative to a no-action scenario. However, with SVE and no cap, the TCE concentration continues to increase for about 15 years relative to the concentration for SVE with no cap. This is because, in the absence of a cap, SVE tends to pull gas phase downward from the atmosphere blocks above, rather than from the sides where the contaminant resides. Meanwhile, the TCE plume at some distance from the SVE well continues to migrate laterally. With a cap in place, gas moves toward the SVE well laterally from all around and hence TCE concentrations immediately decline upon application of SVE to the disposal trenches (Figure 8). The superiority of SVE with a cap for reducing concentrations in the vicinity of the point of extraction is well known. What we have shown is that the beneficial effects of the cap are significant even at the residence 200 m to the west where soil-gas TCE concentrations, and therefore potential health risks due to TCE, would be predicted to decline immediately upon application of SVE.

CONCLUSION

We have shown the preliminary application of T2VOC to the soil-gas transport of TCE in the subsurface. The analysis comprised one part of the SELECT methodology, namely modeling the reduction of TCE concentration under a residence that results from remediation applied 200 m away at the site of TCE disposal. We observed that SVE applied without an impermeable cap over the trenches does not immediately reduce exposure potential, and therefore health risk potential, at the residence. When the disposal trenches are capped, however, TCE concentrations below the residence are immediately reduced upon application of SVE. This analysis required the application of the multiphase transport model T2VOC to link the spatial and temporal evolution of TCE concentrations at the site of disposal and at the off-base residence. The development and integration of all of the components of SELECT, for example, the health risk and financial analyses parts, in conjunction with the multiphase transport piece used in this study, will allow complete analyses that will aid in the selection of remediation schemes that maximize reduction of potential health risk while minimizing costs.

ACKNOWLEDGMENT

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NOTATION

d	ref. TCE diffusivity, $m^2 s^{-1}$
foc	fraction organic carbon
k	permeability, m^2
ppbv	parts per billion by volume
PI	productivity index, m^3
t	time, s or years
ϕ	porosity
τ	tortuosity

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