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A STUDY OF LNAPL MIGRATION THROUGH SOIL CEMENT BARRIER WITH AND WITHOUT FLOW CONDITION

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ABSTRACT

The spill of hydrocarbons from industrial plants is a significant problem for groundwater. Through advection and diffusion, contaminant migration can spread widely in the subsurface. The effect of contaminated groundwater can become still more serious if contamination occurs in sandy soil. This paper focuses on the study of LNAPL migration in soil and through a containment barrier. The simulation study of contaminant migration considers two scenarios, as follows: (1) without groundwater flow and (2) with groundwater flow, with a hydraulic gradient of 0.017. The wall, 5 m deep and 1 m thick, was modeled as a containment system. The NAPL spill was modeled with a constant-rate release lasting 2 years. The study found that the permeability of soil and the hydraulic gradient of the aquifer were the factors that affected contaminant migration. The results obtained could be used as a guide for the design of impervious wall dimensions and properties to properly contain contaminant migration.

INTRODUCTION

Subsurface contamination problems due to the release of toxic substances, such as inorganic and organic compounds including hydrocarbon volatile organic compounds (VOCs), may affect the environment and the life cycle of natural animals and humans.

The spill of light nonaqueous phase liquid (LNAPL), such as gasoline, into the vadose zone is more risky than the spill of heavy contaminants (DNAPL), because LNAPL can spread quickly, especially in the presence of high-permeability soil. For these reasons, this paper focuses on the benzene (STD) migration behavior through a soil cement barrier. Benzene is an aromatic hydrocarbon having a high solubility in water and a non-negligible vapor pressure. When spilled into the subsurface, it migrates, giving rise to multiphase flow processes.

In this study, the simulations took into account different barrier materials and different aquifer hydraulic gradients. The TMVOC simulator was used within the PetraSim 4.2 pre- and postprocessing interface. PetraSim is one of the graphical interface available for the TOUGH2 family of reservoir simulators developed at Lawrence Berkeley National Laboratory (USA). TOUGH2 and its derivatives were recognized for their broad range of subsurface simulation capabilities, including heat and multiphase flow and reactive transport. In the past, modeling of multiphase organic contaminant migration was performed by several authors, such as Abriola and Pinder (1985), Kaluarachchi and Parker (1989), Falta et al.(1995), Soga et al. (2003), Pruess and Battistelli (2003), Fagerlund and Niemi (2003), Dunn (2005), and Battistelli (2008).

SOIL CEMENT COLUMN BARRIER

Soil-cement walls are structures often used to improve the geotechnical properties of soft soil. They can be constructed by two methods: (1) a rotary mixed method, the technique preferred for cohesive soil, with a widespread use in Japan; and (2) a jet grouting method, a technique for both cohesive soil and cohesionless soil. The latter method can be especially useful for sandy soil, where the injection of cement slurry is more effective than in clay. This approach offers the advantage of building wall columns in both a vertical and inclined direction by cement-based grout. The construction of soil-cement columns by means of jet grouting can be depicted step-by-step as shown in Figure 1.

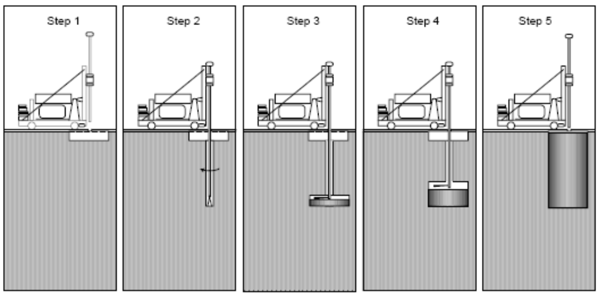

Figure1. Step-by-step construction of soil cements columns by means of jet grouting technique.

In Thailand, soil-cement columns are often used for improvement of soft soil. The main objective is to decrease settlement and increase the baring capacity of soft soil. In addition, they can also reduce the permeability of sandy soil. Therefore, soil-cement columns can also be used as physical barriers to contain the migration of contaminants in the subsurface.

MODELING APPROACH

Model Characteristics and Material Properties

The conceptual models used in the study are shown in Figure 2. They are two dimensional sections 60.2 m long, 15.1 m thick and 1 m wide. The characteristics of the four models are: (1) no groundwater flow (hydraulic gradient equal to zero), (2) groundwater flow with a hydraulic gradient of 0.017 (water table difference of 1 m along a distance of 60 m (1/60), (3) no groundwater flow with containment (hydraulic gradient equal to zero), and (4) ground water flow with a hydraulic gradient of 0.017 with containment. The spill point of the benzene is located in the unsaturated zone at a distance from the left side of 29.6 m for Models 1 and 3, and 19.6 m for Models 2 and 4. The groundwater table is 2 m below the ground surface for Models 1 and 3, while for Models 2 and 4, it is 2 m and 3 m deep at the left and right boundaries, respectively. The containment system is 1 m thick, 5 m deep and is located at 1.5 m from the spill point in the both left and right directions.

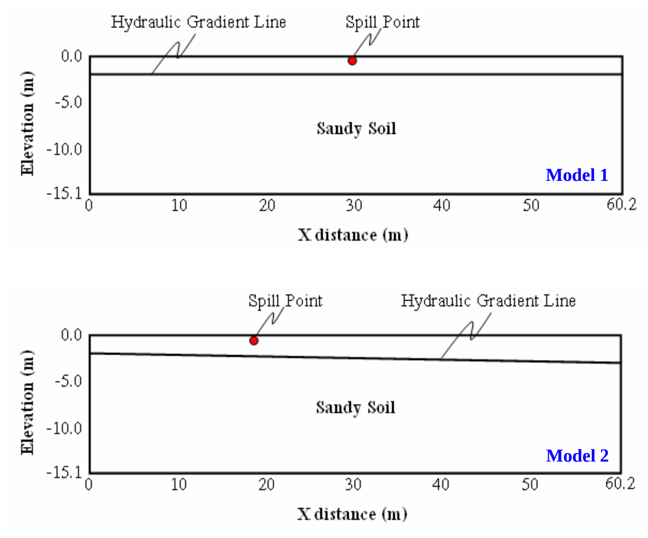

Figure 2. Conceptual models 1, 2, 3, and 4

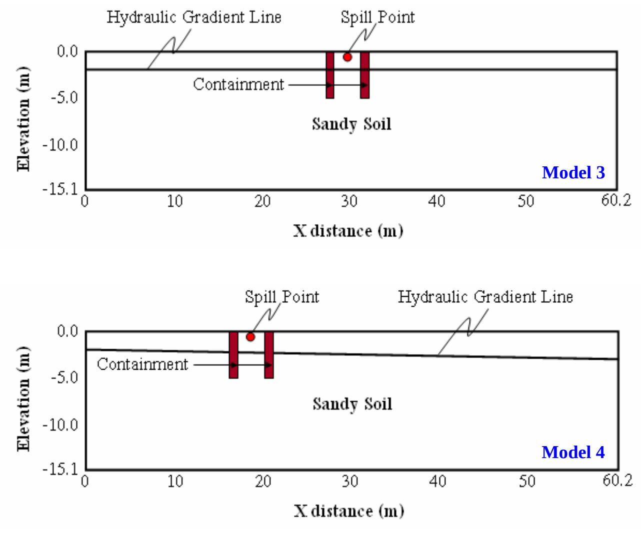

Figure 2. Conceptual models 1, 2, 3 and 4 (Con.)

We studied the effect of intrinsic permeability. Three intrinsic permeability values of soil were used: 10^{-9} m^2, 10^{-10} m^2 and 10^{-11} m^2. Three intrinsic permeability values of the barrier were also used: 10^{-13} m^2, 10^{-14} m^2 and 10^{-15} m^2. This study considers a total of 24 different cases; basic petrophysical properties are listed in Table 1. The relative permeability and capillary pressure curves for three-phase systems are described according to the Stone (1970) and Parker et al. (1987) models, respectively. The corresponding parameters are summarized in Tables 2 and 3 for the relative permeability and the capillary pressure, respectively. The simulations are performed at a constant temperature of 20°C. The atmospheric boundary conditions are fixed at the grid top and specified as a constant absolute pressure of 1.01×10^5 Pa.

Table 1. Main petrophysical properties of rock domains

Soil criteria	Rock grain density kg m^{-3}	Porosity	Horizontal permeability m^2	Vertical permeability m^2
ATMOS	2600	0.35	$1x10^{-8}$	$1x10^{-8}$
Soil 1	2600	0.31	$1x10^{-9}$	$1x10^{-9}$
Soil 2	2600	0.35	$1x10^{-10}$	$1x10^{-10}$
Soil 3	2600	0.39	$1x10^{-11}$	$1x10^{-11}$
Wall 1	2600	0.43	$1x10^{-13}$	$1x10^{-13}$
Wall 2	2600	0.47	$1x10^{-14}$	$1x10^{-14}$
Wall 3	2600	0.51	$1x10^{-15}$	$1x10^{-15}$

Table 2. Relative permeability parameters of different rock domains (first Stone's modified model)

Soil criteria	Swr	Snr	Sgr	n exponent
ATMOS	0.15	0.05	0.05	3
Soil1,Wall1	0.15	0.05	0.05	3
Soil2, Wall2	0.15	0.05	0.05	3
Soil3, Wall3	0.15	0.05	0.05	3

Remarks: Swr = irreducible aqueous phase saturation, Snr = irreducible NAPL saturation, Sgr = irreducible gas phase saturation, NAPL = non aqueous liquid

Table 3. Capillary pressure parameters of different rock domains (Parker's model)

Soil criteria	Sm	αgn	αnw	n exponent
ATMOS		no capillary		
Soil 1	0	100	110	1.84
Soil 2	0	30	33	1.84
Soil 3	0	10	11	1.84
Wall 1	0	1	1.1	1.84
Wall 2	0	3	3.3	1.84
Wall 3	0	0.1	0.11	1.84

Remarks: Sm = limiting saturation, αgn = strength parameter for gas-NAPL, αnw = strength parameter for NAPL-aqueous phase liquid

The applied boundary conditions are shown in Table 4. For this application, the formation of heterogeneities, the seasonal water table fluctuations, and the water infiltration have been neglected.

Table 4. Boundary conditions applied to simulation

Boundary	Pressure	Condition
Hydraulic Gradient, i = 0		
Top	$1.01x10^5$	Gas Only
Left	$1.01x10^5$	Gas and Water, Above
(x = 0 m)	$1.01x10^5$+ 9789z	Water Table (z <= 2.1 m, water sat. = 0.20)
		Water Only, Below Water Table (z > 2.1 m)
Right	$1.01x10^5$	Gas and Water, Above
(x = 60.2 m)	$1.01x10^5$+ 9789z	Water Table (z <= 2.1 m)
		Water Only, Below Water Table (z > 2.1 m)

Table 4. Boundary conditions applied to simulation (Con.)

Boundary	Pressure	Condition
Hydraulic Gradient, i = 0.017		
Top	$1.01x10^5$	Gas Only
Left	$1.01x10^5$	Gas and Water, Above
(x = 0 m)	$1.01x10^5$+ 9789z	Water Table (z <= 2.1 m, water sat. = 0.20)
		Water Only, Below Water Table (z > 2.1 m)
Right	$1.01x10^5$	Gas and Water, Above
(x = 60.2 m)	$1.01x10^5$+ 9789z	Water Table (z <= 3.1 m)
		Water Only, Below Water Table (z > 3.1 m)

Model Characteristics and Material Properties

The modeling is discretized with 16 layers and 62 columns for a total of 992 elements. The vertical and horizontal spacing is 1×1 m, except the elements of top row which are 1×0.1 m; left and right boundary columns have the spacing of 0.1×1 m. The simulations are divided into several steps, as follows: (1) setting up the initial conditions at left and right boundary columns; (2) running to steady state controlled by gravity and capillary forces and subjected to the boundary conditions at lateral and top grid sides specified for each case; and (3) modeling of spill for 2 years, starting from the steady-state conditions obtained in Step 2. The LNAPL spill has been modeled assuming a constant rate of 1.154×10^{-5} kg/s, equivalent to 1 kg/day. In this study, the effectiveness of the barrier is analyzed, looking at the effects of aquifer permeability and hydraulic gradient.

RESULTS

Modeling of steady state

The initial conditions for modeling the spill scenarios were obtained running the system to steady state, governed by gravity and capillary forces under the boundary conditions specified for each case. The steady-state pressure distribution is shown in Figure 3. In case of i = 0, the LNAPL plume spreads symmetrically over the water table, while in the case of aquifer flow, the LNAPL plume moves preferentially following the water table slope.

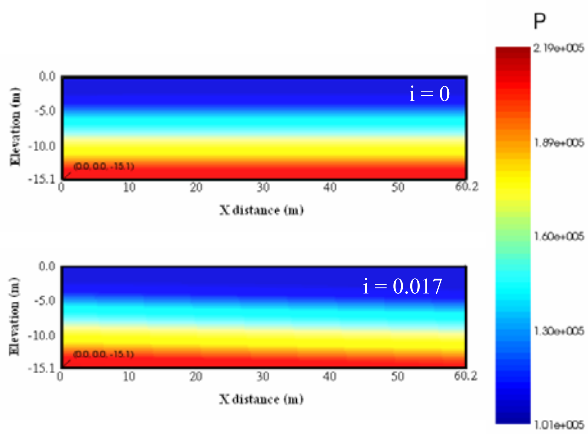

Figure 3. Pressure distribution at steady state conditions.

Migration of LNAPL into subsurface

The spill of benzene was modeled at a constant rate of 1 kg/day into the vadose zone for 2 years. The simulations were performed under isothermal conditions. In this study, the standard benzene properties (STD) supplied by Petrasim have been used. The diffusion coefficients of mass components in the different phases are summarized in Table 5.

Table 5. Molecular diffusion coefficients of mass components.

	GAS	AQUEOUS	NAPL
Air	2.0×10^{-5}	6.0×10^{-10}	6.0×10^{-10}
Water	2.0×10^{-5}	6.0×10^{-10}	6.0×10^{-10}
Benzene	7.7×10^{-6}	6.0×10^{-10}	6.0×10^{-10}

The simulation results relative to the total mass fraction of benzene in the aqueous liquid (XVOCW) can be described as follows:

(1) Case i = 0: the benzene moves downward according to gravity; then the LNAPL plume floats on the water table and spreads out laterally. The depth reached by the dissolved benzene plume below the water table is about 1.5 m, and the distance of the benzene migration decreases with the soil permeability. In the presence of the containment wall, the dissolved benzene is contained by the barrier and cannot migrate beyond the containment.

(2) Case of i = 0.017: once it reaches the water table, the LNAPL plume migrates preferentially in the direction of water table gradient. The shape of the dissolved benzene plume changes, depending on the soil permeability. The result of the model scenario without containment shows that if the permeability of soil decreases, the LNAPL plume could migrate to longer distances. Higher soil permeability allows a greater evaporation of benzene. The results of the model scenario with wall containment show that the benzene migration is reduced by the containment. The dissolved benzene plume moves downward along the barrier, and some benzene can flow under the wall base when the soil has lower permeability, as shown in Figure 4 and 5.

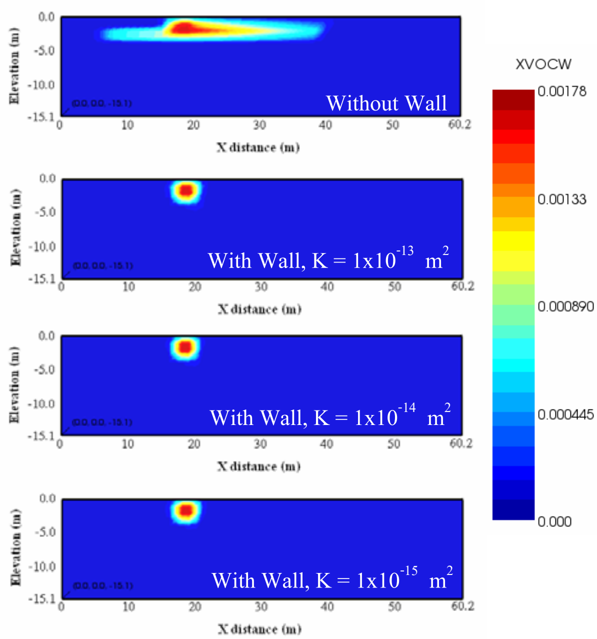

Figure 4. Total mass fraction of VOCs in aqueous phase in sandy soil with K = 1×10^{-9} m^2 and i = 0.017.

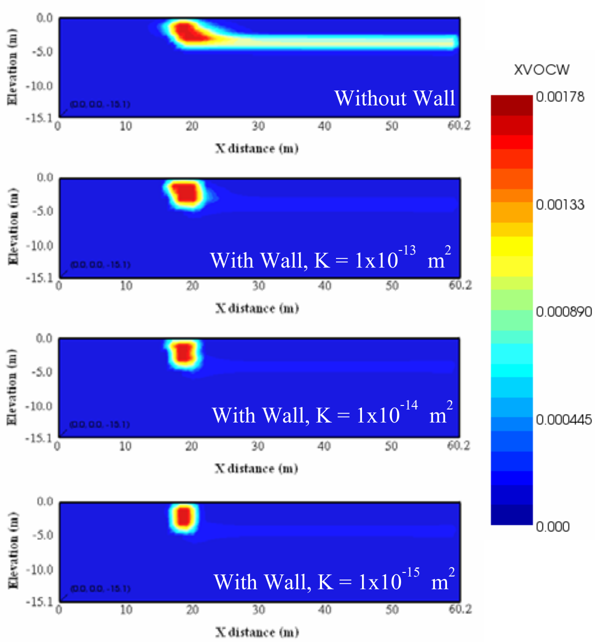

Figure 5. Total mass fraction of VOCs in aqueous phase in sandy soil with K = 1×10^{-11} m^2 and i = 0.017.

The total mass fraction of VOCs dissolved in the aqueous phase outside the containment zone, at depth of 1–6 m below the ground surface in the case of i = 0 with containment, is reduced close to zero, as shown in Figures 6–8. For the case of i = 0.017, the concentration of the benzene increases at the end of the barrier in concert with the permeability decrease, due to the effect of groundwater flow, as shown in Figures 9–11.

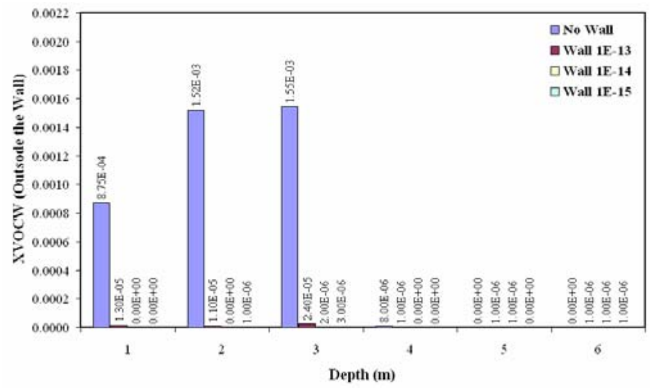

Figure 6. Comparison of total mass fraction of VOCs in aqueous phase outside the wall for sandy soil layer with K = $1x10^{-9}$ m^2 and i = 0.

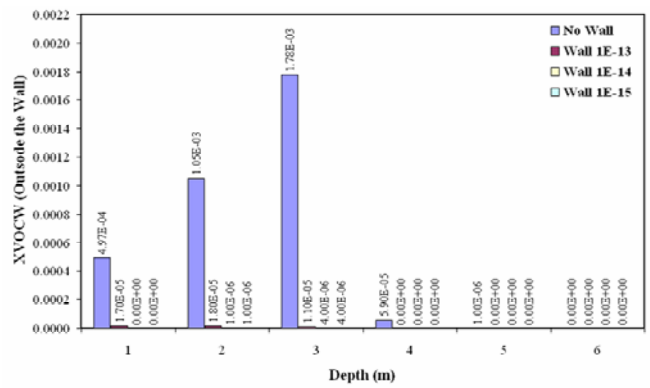

Figure 7. Comparison of total mass fraction of VOCs in aqueous phase outside the wall for sandy soil layer with K = $1x10^{-10}$ m^2 and i = 0.

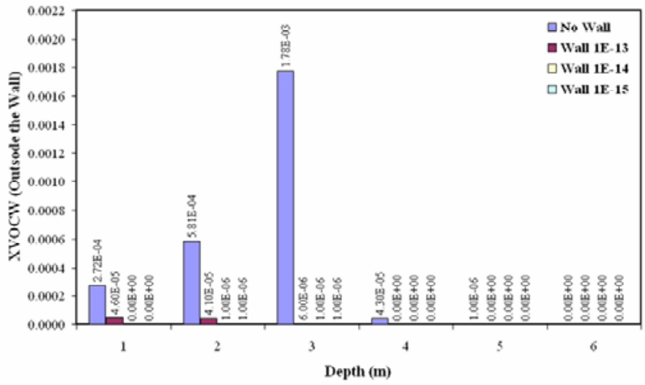

Figure 8. Comparison of total mass fraction of VOCs in aqueous phase outside the wall for sandy soil layer with K = $1x10^{-11}$ m^2 and i = 0.

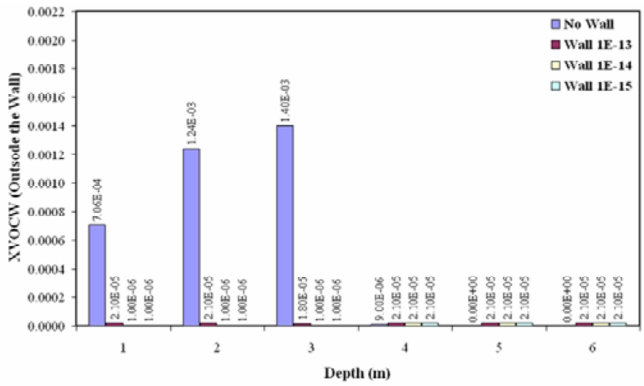

Figure 9. Comparison of total mass fraction of VOCs in aqueous phase outside the wall for sandy soil layer with K = $1x10^{-9}$ m^2 and i = 0.017.

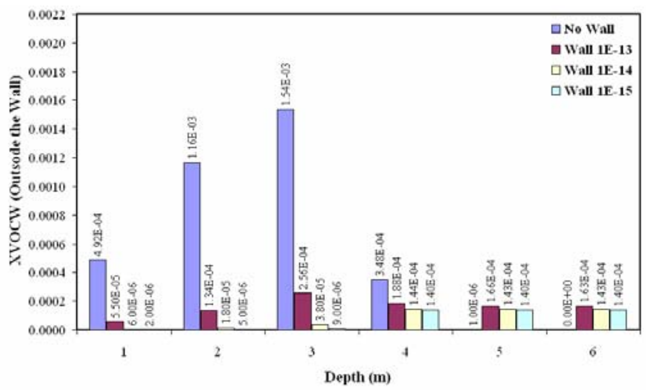

Figure 10. Comparison of total mass fraction of VOCs in aqueous phase outside the wall for sandy soil layer with K = $1x10^{-10}$ m^2 and i = 0.017.

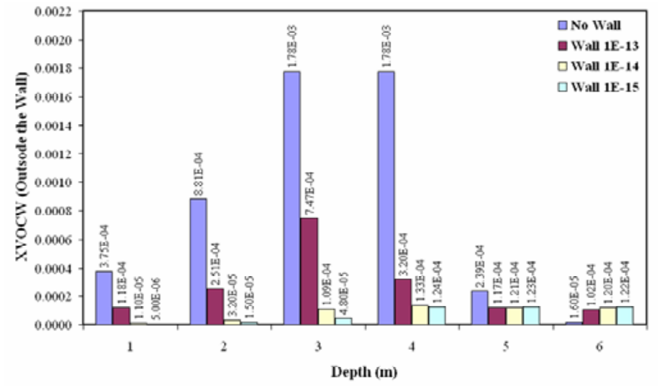

Figure 11. Comparison of total mass fraction of VOCs in aqueous phase outside the wall for sandy soil layer with K = $1x10^{-11}$ m^2 and i = 0.017.

CONCLUSIONS

This paper presents simulation of benzene migration in the subsurface as a consequence of a constant-rate spill in the unsaturated zone. Several scenarios have been modeled with a phreatic aquifer in a sandy soil of varying permeability, with different hydraulic gradients, and with or without the presence of a vertical containment wall. Simulations results reveal that the soil-cement barrier can reduce the contamination of the benzene and show that soil permeability and water table hydraulic gradient are the significant factors.

The benzene migration in the case of i = 0, occurs only by a gravity-driven NAPL plume flow and diffusion of dissolved benzene in the groundwater. In the presence of aquifer flow, dissolved benzene may be transported over long distances by advective flow. Without the groundwater flow, the contaminant migration is contained by the soil-cement barrier in the vadose zone; the dissolved benzene plume reaches less than 2 m below the water table. Consequently, the depth of the soil-cement wall should be more than 2 m below the groundwater level. With groundwater flow, the concentration of contamination depends on the hydraulic gradient, which enhances the transport processes. The hydraulic gradient has an impact on the depth of contaminant migration outside the wall. From the scenarios simulated, it can be concluded that soil-cement barriers can be used to limit the spread of benzene spilled in the unsaturated zone. Modeling studies such as those described may help in the design of containment operations and in risk assessment studies.

Note that presented herein is a preliminary study dealing with the processes controlling the migration of VOCs spilled in the vadose zone in the presence of vertical containment walls in sandy aquifers. The properties of the soil-cement used in these simulations are derived from bibliographic sources. Experimentally derived properties will be considered in future simulation works.

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