Soil vapor extraction of chlorinated solvents at an industrial site in Brazil

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Abstract

This study presents the design, monitoring and remediation strategy for a soil vapor extraction (SVE) system installed at an industrial site contaminated with a mixture of organic compounds, in particular 1,2 dichloroethane, carbon tetrachloride and chloroform. The unsaturated zone at the site is very deep and presents near ideal conditions for SVE, with the contaminated portion of the porous media characterized by alluvial deposits of a well graded sand followed by a capillary barrier at 28 m of depth, which limited DNAPL downward migration. The soil cleanup time and the optimal removal rates of mass, considering different values of vacuum/discharge applied in the SVE system, have been estimated through the use of numerical sensitivity analysis. Results of the pilot-scale testing activities allowed for the calibration of flow and contaminated mass transport models and the determination, in a preliminary phase, of the infiltrated mass of different compounds.
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1. Introduction

The off-site migration of groundwater impacted by non-aqueous phase liquids (NAPLs) is a major concern since it may pose serious risk to human health, safety and the environment. A common and efficient alternative of treating unsaturated soils impacted by volatile and semi-volatile organic chemicals (VOC) is through the use of soil vapor extraction (SVE), which may also be used in association with biodegradation processes such as bioventing. Advancements of in situ bioremediation techniques have demonstrated that SVE technologies may significantly enhance and sustain the aerobic bioremediation processes by providing oxygen to the soil microorganisms. The advantages of SVE systems over other remediation technologies may be attributed to its relative low cost and relative simplicity of installation, system operation and minimal amount of equipment required [1]. Another advantage of this technology is that mitigation is completed in situ, reducing the risk of the general public to the toxic compounds. Soil remediation utilizing the SVE system may also be installed in parallel to other remedial methodologies, in case the saturated zone is also impacted by the vertical migration of organic compounds denser than

water (DNAPLs). The success of the SVE system, however, is mostly a function of an adequate air movement within the contaminated portion of the subsurface [2].

Toxic organic compounds that are spilled into the subsurface are subjected to a series of chemical and physical transformations. In the unsaturated zone, the infiltrating pure phase product may stop its downward migration due to the existence of a low permeability stratum and form an immobile residual source. Part of the volatile contaminant evaporates and migrates through the processes of diffusion. As the vapors migrate, they dissolve into the soil moisture, and may be sorbed onto the soil particles. Part of the contaminant mass will be passively lost to the atmosphere in the case of an open ground surface. The contaminants may also be flushed deeper into the saturated zone by infiltrating storm water and form a dissolved phase in groundwater. Subsequent transport in those phases may cause widespread groundwater contamination. All of these processes are driven by natural forces such as gravity or infiltrated rain.

The performance of an SVE system depends on properties of both the contaminants and the soil. Two major physical mechanisms are observed in SVE operations: mass transfer, the partition of one phase to another, and mass transport. Volatile and semi-volatile compounds will enter the vapor phase by evaporating from the pure phase liquids or volatilizing from the soil moisture. Desorption from the soil particles may occur as well. The rate of mass transfer will depend

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on a series of variables such as subsurface temperature, soil humidity and contaminant properties including solubility, vapor pressure and density. Mass transport is the second process enhanced by the SVE system. The movement of vapor in the subsurface is caused primarily by advection, which is related to the existence of pressure gradients that are developed during the operation of vapor extraction wells. Vapor transport is dependent primarily on subsurface parameters such as soil permeability and humidity as well as on the magnitude of vacuum pressure imposed by the SVE system.

The purpose of this paper is to investigate, through the use of numerical sensitivity analysis, parameters that are essential to an adequate operation of a SVE system, such as soil cleanup time and the optimal removal rates of mass, considering different values of vacuum/discharge applied to system. It is known that the time required to clean the site using vapor extraction technology depends not only on the amount, nature and distribution of contaminants in the subsurface, but also upon the rates at which mass transfer and mass transport occur [3]. The spatial distribution of the intrinsic soil permeability exerts great influence on the performance of vapor extraction operations as well, mainly in the vicinity of the infiltrated NAPL. The existence of surface cover at the site may also contribute to reduce cleanup time by improving the distribution of contaminated air flow through the flow field. The process schematic of a SVE system is depicted in Fig. 1.

The scope of this paper is limited to vapor flow and transport in the unsaturated zone in the presence of an immobile soil moisture phase. The vapor is assumed to originate at an immobile source of organic liquid in the form of residual phase or "pool" of DNAPL, located at the vicinity of a single extraction well. The application of external pressure gradients at the well (vacuum pressure) causes contaminant vapor movement and consequent removal by the SVE system. The governing equations that describe isothermal multiphase flow and transport in the subsurface are complex

and must include the flow of water, gas and oil phases, partitioning of species between these phases, and transport of species in each of the phases [4].

2. Model conceptualization

The volatile organic compounds are assumed to be present in the solid adsorbed phase as well as three fluid phases: gaseous, organic (NAPL) and aqueous phases. The organic and aqueous liquid phases are assumed to be stagnant, whereas the advective and diffusive fluxes are related to the gaseous phase containing air components as well as the toxic gases. The mathematical formulation of subsurface contaminant vapor plumes is obtained by solving the partial differential flow and transport equations, subjected to boundary and initial conditions. The general mathematical equations describing fluid and mass transport in porous media are applicable to both the gaseous and aqueous phases and may be found in [5].

Fluxes in the gaseous phase result from pressure gradients imposed by the SVE well, consisting of advective and diffusive mass fluxes for each component—air and the volatile organic compounds. The general gas flow equation that describes the distribution of gas pressure in the unsaturated zone is deducted by substituting expressions for the fluxes in the gaseous phase into the mass balance equations for the air component and also for each organic compound.

The advective–diffusive transport equation for each volatile organic compound is obtained by substituting the mass balance equations for each compound in the gaseous, aqueous and solid phases into the equations of gas mass flux associated with the volatile organic and the air component. Vapor concentration gradients are used in the diffusive/dispersive fluxes instead of gradients of mass.

Mass removal of NAPL is physically controlled by a series of elements specific to the site/contaminant nature as well as the SVE operational parameters. These include the magnitude of pressure gradients imposed by the SVE well for a given discharge; the distribution of NAPL in the subsurface; concentration gradients near the contaminant phase and the contaminant vapor pressure in order to favor NAPL partitioning and mass transfer; the soil air permeability, porosity and moisture; and also the existence of a soil cover at the ground surface. These elements will determine, in different levels, the successfulness of the SVE operations.

The numerical model AIRFLOW/SVE [6] was utilized, which is two-dimensional finite-difference numerical model that describes the movement of volatile organic chemicals in unsaturated soil, in response to the application of a vacuum pressure at the vapor extraction well. It is a cylindrical model, or rather, it assumes gas flow and vapor transport to be treated as axi-symmetric processes with respect to the extraction well, simulating gas flow and transport in the radial and vertical directions. It allows for mass removal of NAPL based upon a given air flow configuration, obtained by the
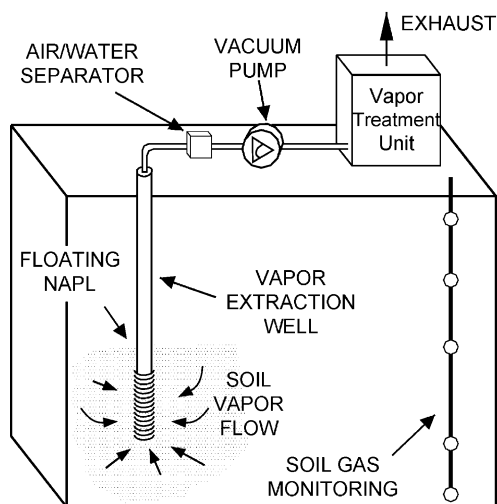

Fig. 1. Process schematic of a soil vapor extraction system.

steady-state flow model simulation. The model is limited to a single extraction well and is well suited for a pilot test phase, as was applied in this work.

3. Physical setting

The SVE model was applied to a geological setting located in a humid and tropical region in Brazil. The geometry of the domain corresponds to a two-dimensional axi-symmetric system with a single SVE well. Model domain included an area of approximately 1960 m^2 and was initially divided into 1960 finite difference blocks of 1 m^2, as illustrated in Fig. 2. Additional blocks were added to the domain in order to precisely represent significant pressure gradients developed at the vicinity of the extraction well. A schematic representation of the simulation domain is depicted in Fig. 3 along with the boundary conditions for flow and transport models.

The ground surface is assumed to be covered and impervious. The spatial domain extends from ground surface to a depth of 28 m, with the lower boundary represented by a clay layer impervious to vapor flow. The left-hand boundary represents the soil vapor extraction well. The screened portion is defined as a specified-pressure boundary while the non-screened interval (well casing) is impermeable, and is represented by second-type boundary conditions for both flow and transport. The right-hand boundary represents the radius of influence of the vacuum extraction well and is specified as a fixed-pressure boundary at atmospheric pressure and zero concentration.

The conceptual model was divided into two geological layers, according to Fig. 2. The first was a sandy clay with 10 m of depth followed by a well-graded sand extending to the bottom domain at 28 m. The covered ground surface as well as the top clay layer acts as an impediment to vapor loss to the atmosphere, facilitating its removal by the SVE well.
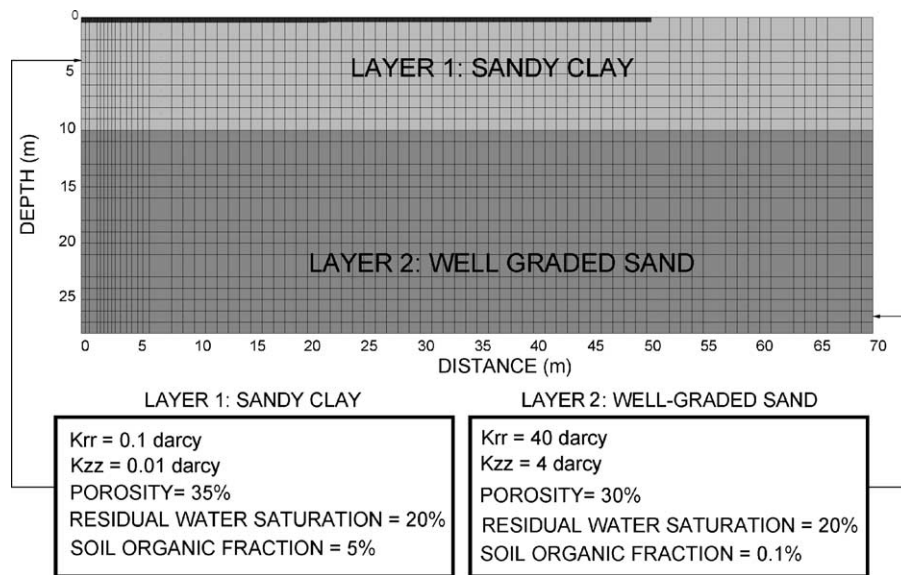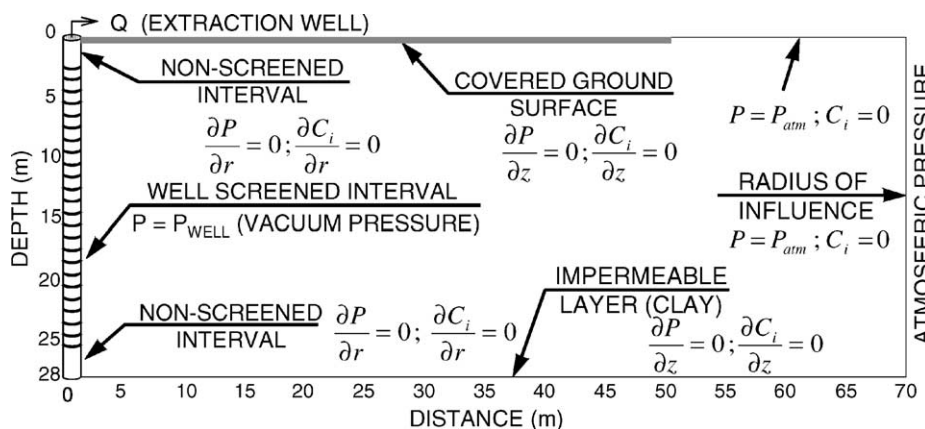

Fig. 2. Finite difference grid.

Fig. 3. Simulation domain and boundary conditions.

Table 1
Simulation parameters

Parameter	Value
Length of flow field in x direction	70 m
Depth of flow field in z direction	28 m
Number of blocks in the x direction	70 m
Number of blocks in the z direction	28
Block size in x and z direction	1 m
Total number of cells	1960
Prior mean permeability of sand	40 darcy (3.95×10^{-11} m^2)
Air conductivity	2.52×10^{-5} m/s
Porosity of sand (assumed typical value)	0.3
Depth of well screen	1.5–25.5
Extraction flow rate	197 m^3/h
Vacuum air pressure	2.0 kN/m^2
Residual water saturation	0.2
Soil organic fraction	0.001
Gas (air) density	1.205 kg/m^3

The physical properties for the domain as well as simulation parameters are summarized in Table 1. Moisture content throughout the unsaturated zone was assumed to be uniform at a residual capacity of 20% of bulk volume. Model properties presented at Table 1 are the ones resulted from the flow model calibration process that was conducted previously.

The source of toxic vapors was attributed to a surface spill of a mixture of organic compounds, in particular chlorinated solvents. Throughout the domain, the source of organic compounds vaporizes, generating a flux of vapor flow that mixes with air and migrates through the pores spaces toward the SVE well. The real system is approximated with the idealized axi-symmetric system in Fig. 4, which illustrates the geological setting as well as the NAPL distribution at the unsaturated zone.

It is assumed that the residual liquid solvent penetrated to a depth of 28 m and the impermeable clay layer at the bottom domain limited its downward movement. The source is assumed to be present in both residual form as well as a floating NAPL present on top of the impervious layer.

Due to different concentration values found during monitoring, the percentage of contaminants in the mixture was specified as follows: 90% 1,2 dichloroethane, 5% carbon tetrachloride, 5% chloroform. All components are DNAPLs with relatively high vapor pressures and low adsorptive properties, which are favorable to SVE operations [7]. The NAPL distribution present in Fig. 4 is one of the many different settings that were idealized during model sensitivity analysis, relative to a mass of 450 t [8]. For each distribution scenario, different values of residual NAPL saturation were attributed to the contaminant source (not shown here).

4. Model calibration

Several vapor extraction wells were executed at the site in order to identify areas with different contaminant concentrations at the unsaturated zone. The well VEW-04 was located at the most contaminated area and was the chosen well to initialize the pilot test process and model sensitivity analysis. The flow model for that well was calibrated for the conditions of the pilot test results conducted in a preliminary phase of the remediation program.

The steady-state flow model results for the field conditions of discharge and pressure equal to 197 m^3/h and 2 kN/m^2 ($\sim$200 mm H$_2$O), respectively, are illustrated in Fig. 5. Model parameters were adjusted during the calibration process in order to reproduce field data. The calibrated intrinsic horizontal permeability of the sand layer was 40 darcy or 3.95×10^{-7} cm^2. This is equivalent to a value of air conductivity equal to 2.52×10^{-5} m/s for that layer. Fig. 6 illustrates the pilot test results—vacuum pressure distribution—for the vapor extraction well VEW-04, for the same conditions above, in order to obtain the well radius of influence and define model spatial domain. Significant pressure gradients are developed in the first five meters from the extraction well, for that applied vacuum pressure, as expected. The radius of influence as well as soil gas permeability are key parameters for evaluating technical feasibility of SVE systems and
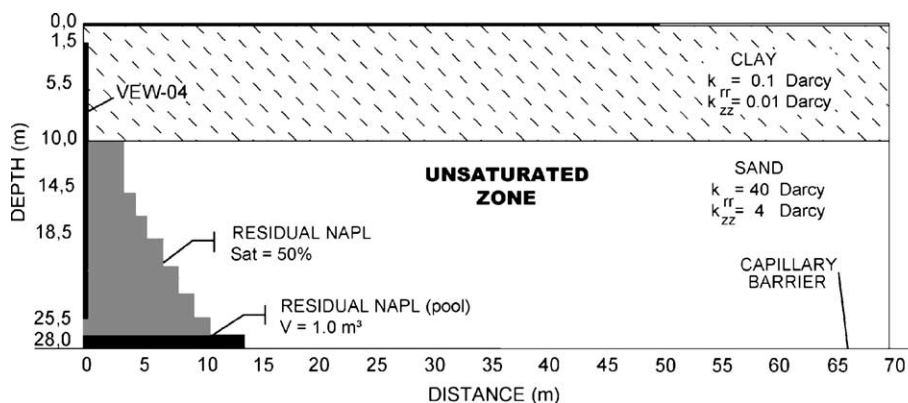

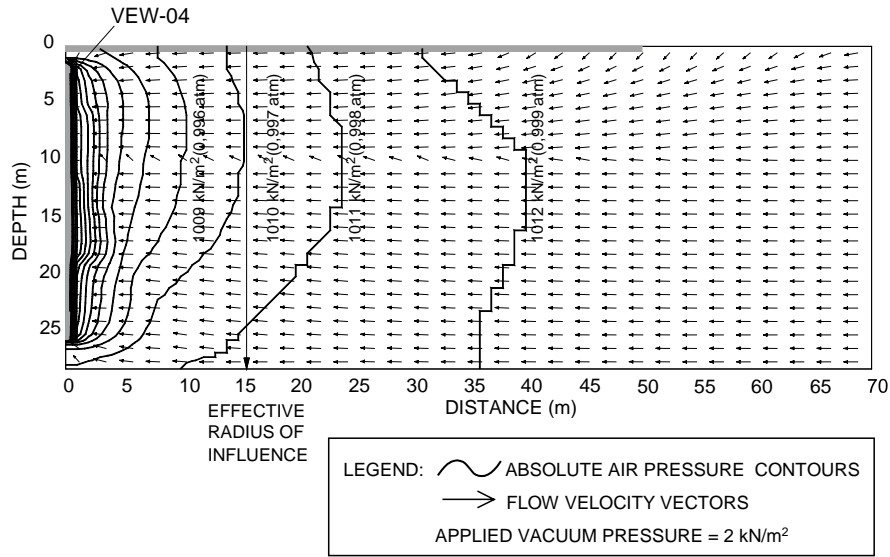Fig. 4. NAPL distribution at the unsaturated zone.

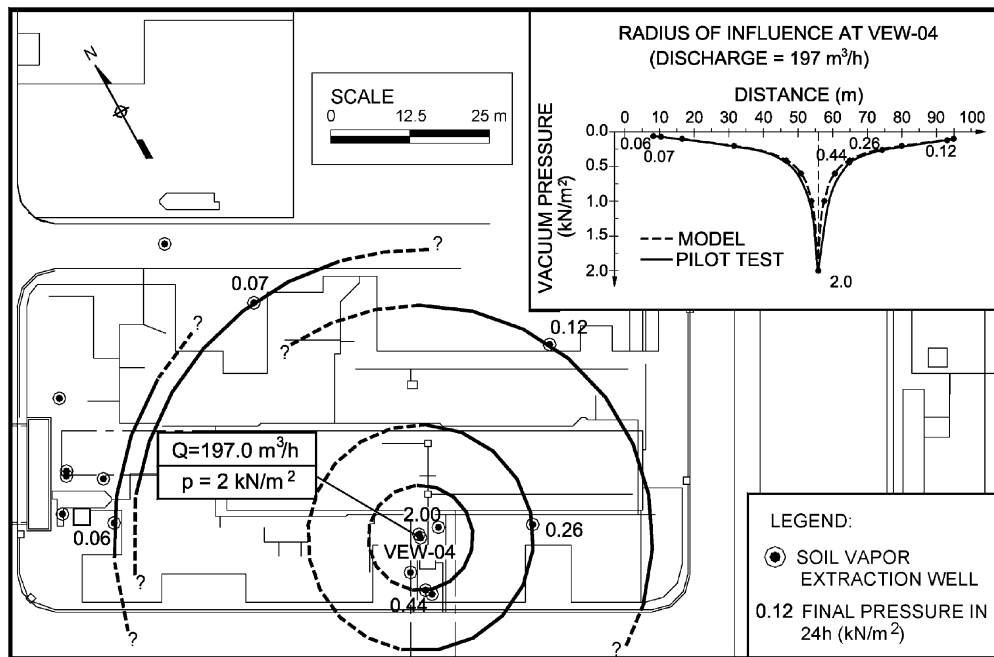Fig. 5. Steady-state pressure distribution at VEW-04.

Fig. 6. Radius of influence for VEW-04 (pilot test).

providing system data. The calculated radius of influence was 22 m, based on a "cut-off" vacuum level of 10% of the applied vacuum at the extraction well. A practical effective radius of 15 m was suggested for this site due to variations in the values of vacuum pressure along with testing procedures.

5. Mass removal performance

The mass transport model simulations included many different distributions of NAPL in the unsaturated zone. The variation of field concentration values with time, for the

VEW-04, were compared to calculated concentration values for the transport model to predict the approximate mass of contaminants that was present in the subsurface at the unsaturated zone. The analytical field data were obtained for a period of approximately 9 months, from May 2001 to February 2002.

Different mass distributions were related to different amounts of infiltrated mass of DNAPLs. Model calibration results are presented in Fig. 7, for five different masses of contaminants, ranging from 90 to 660 t. It is verified that an adequate adjustment of field data was obtained for
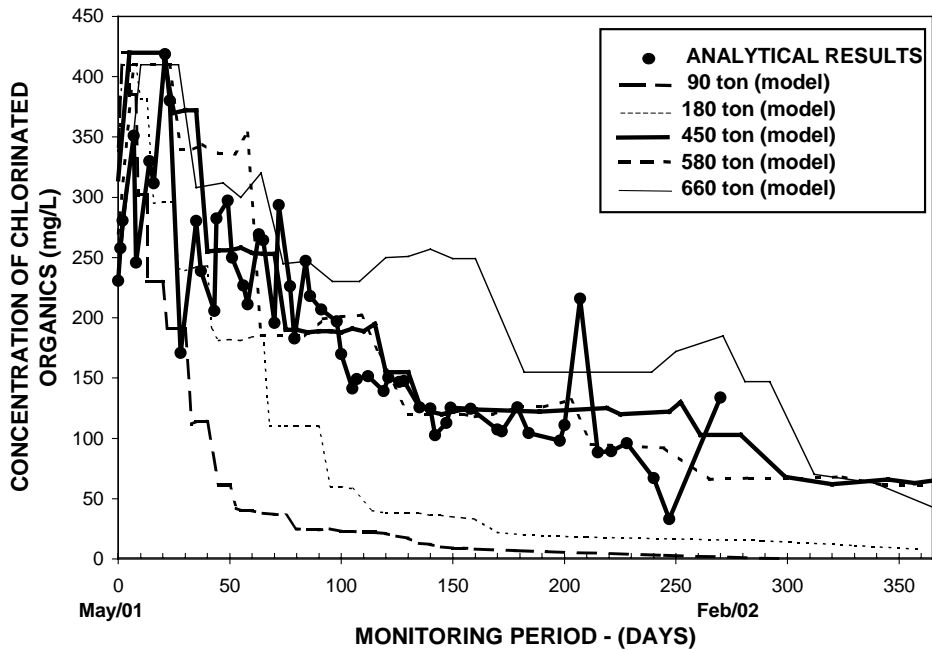
Fig. 7. Decreasing concentration profile for VEW-04, for different values of infiltrated mass.

simulated masses between 450 and 580 t of contaminants. Considering an amount of 450 t, for instance, it has been verified that 46% of the infiltrated mass—about 206 t was extracted from subsurface during the 9-month extraction period from a single well. A final total concentration of about 80 mg/L has been observed from soil gas samples at VEW-04. Fig. 8 presents the cumulative mass removal over time during pilot test at VEW-04. An average mass removal rate equal to 23 t per month was obtained.

Figs. 9 and 10 present, respectively, the concentration levels in years 2000 and 2002 for the unsaturated zone at the site. The figures indicate two major contaminated portions at the site, where pilot tests have been conducted, decreasing contaminant concentrations in a significant manner. Initial concentrations in the order of 1000 mg/L have reduced to values smaller than 100 mg/L at the site. A total mass removal equal to 206 and 65 t was possible from VEW-04 and VEW-01, respectively, as indicated in Fig. 10. The modeling
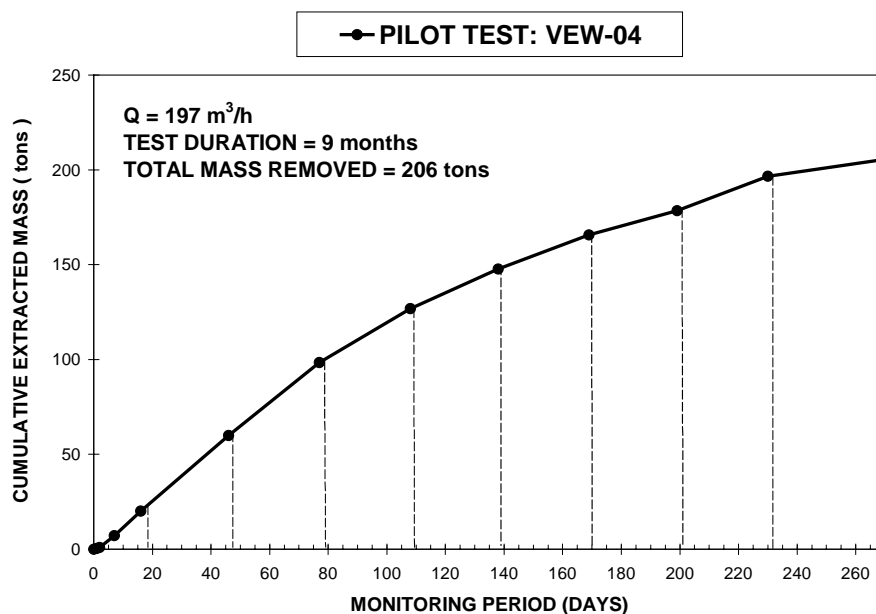

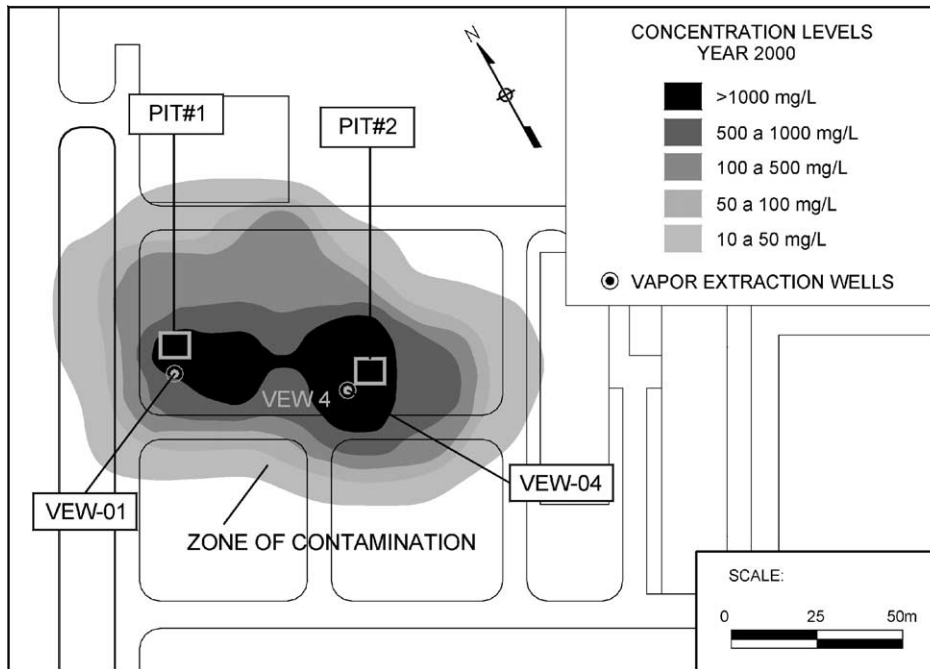Fig. 8. Cumulative mass removal during pilot test at VEW-04.

Fig. 9. Concentration levels at the unsaturated zone (year 2000).

study presented here was conducted for the contaminated area of the unsaturated zone beneath PIT#2.

6. Sensitivity analysis

A sensitivity analysis was performed in order to gain insight into the processes and parameters influencing the field results. This analysis was conducted for two different group of parameters: site/contaminant parameters and design parameters for SVE operations. These included soil gas permeability, contaminant distribution in the subsurface, ground surface cover and well discharge/vacuum pressure. The sensitivity analysis for the design parameters was essential to obtain soil cleanup time for different conditions. The time required to remove all mass from the unsaturated
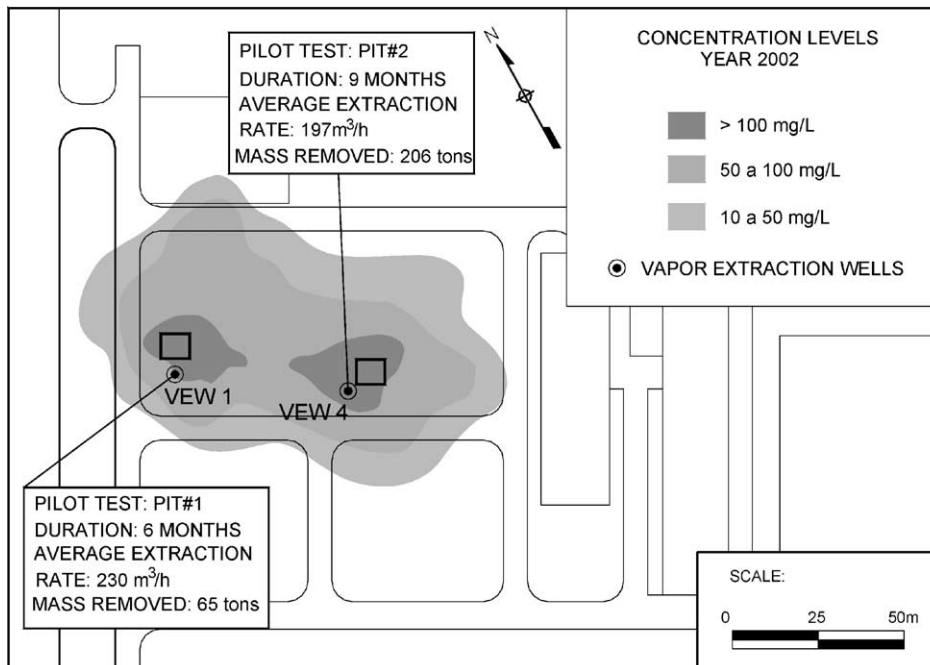

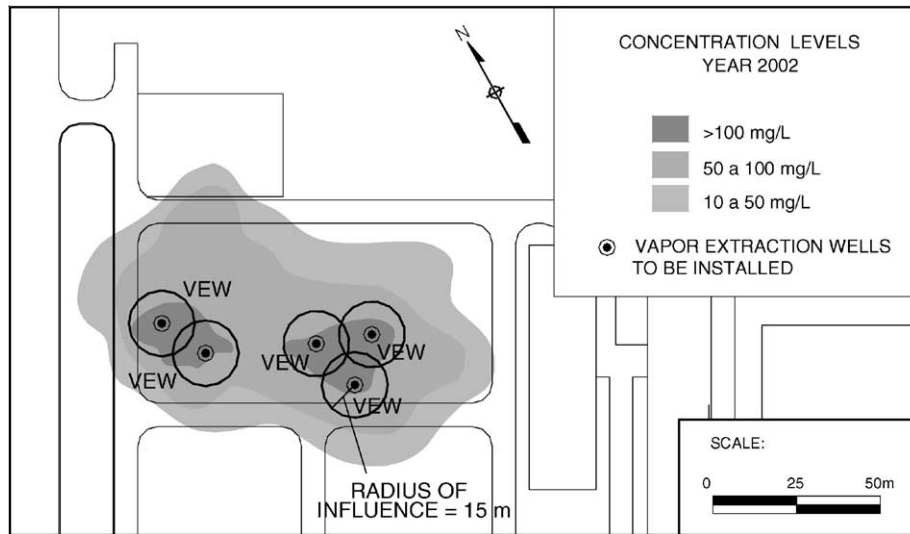Fig. 10. Concentration levels at the unsaturated zone (year 2002).

Fig. 11. Suggested full scale SVE systems to be installed.

zone depends upon two components: the time needed to volatilize all residual NAPL and the time required for the volatilized contaminant to migrate form the NAPL source to the SVE system. Usually, mass transport time is much smaller than the time for volatilization. Therefore, cleanup time is mostly a function of that later process.

It has been observed that variations in soil permeability produce a significant impact on transport mechanisms and therefore on soil cleanup time. SVE systems should be preferentially used in cases of medium to coarse sand, where the process of advection prevails. For soils with permeabilities equal to 4 darcy—1 order of magnitude lower than the real system in Table 1, it has been verified an increase of about 80% for the soil cleanup time for the distribution of Fig. 4.

The effectiveness of soil covers depends on the distribution of the contaminants at the subsurface. In this present case, the existence of a surface cover on the upper boundary domain did not alter soil cleanup time in a significant way. This is due to mass distribution of contaminants, concentrated mostly on the lower boundary domain.

The effects of different applied vacuum pressures/discharges on soil cleanup times are summarized in Table 2, for a

10-year period. Using a discharge of 197 m^3/h, for instance, it has been verified that 97% of the infiltrated mass would be removed in 10 years of continuous application of the SVE system using a single well. The application of higher removal rates would not increase, in a significant manner, this percentage, due to the difficulties of removing the residual mass still present in the unsaturated zone. Two or three wells working together would certainly provide better results in terms of mass removal rates. Using a system with three extraction wells, located at PIT#2, as in Fig. 11, with a screen interval of approximately 12 m, the well extraction air flow rate was estimated as $Q_{well} = 0.3\,m^3$/m min or $Q_{well} = 216.0\,m^3$/h for each well, based on the air flow generation plot of Fig. 12 (adapted from [2]).

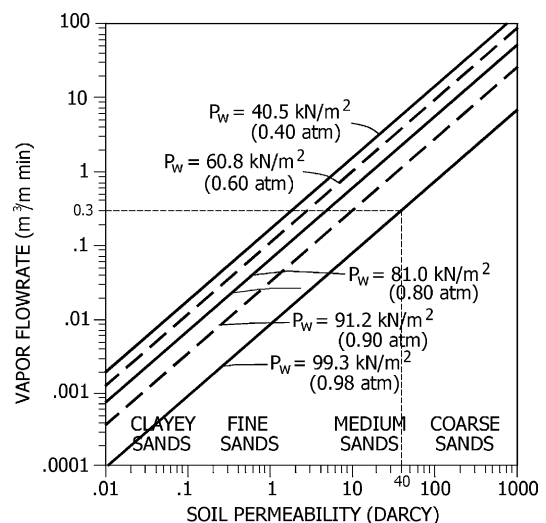Is has also been verified a maximum variation of 30% in soil cleanup times for the cases where it was considered

Table 2
Percentage of contaminant mass removed from soil, for an infiltrated mass of 450 t

Period	Scenario 1 ($Q = 104\,m^3$/h; $p = 1\,kN/m^2$) (%)	Scenario 2 ($Q = 197\,m^3$/h; $p = 2\,kN/m^2$) (%)	Scenario 3 ($Q = 460\,m^3$/h; $p = 3.5\,kN/m^2$) (%)
9 months	31	46	63
1 year	42	64	76
2 years	63	78	89
5 years	82	93	96
10 years	94	97	98

Fig. 12. Air flow generation plot (adapted from [2]).

equal masses of infiltrated NAPL, with different NAPL distributions in the unsaturated zone.

7. Conclusions

The soil cleanup time and the optimal removal rates of mass, considering different values of vacuum/discharge applied in the SVE system, have been estimated through the use of numerical sensitivity analysis for a specific case study. It has been observed that the site cleanup time using soil vapor technology depends not only on the amount, nature and distribution of contaminants in the subsurface but also on the mass transfer and mass transport mechanisms. In addition, geological features play an important role on SVE performance. The spatial distribution of the soil permeability, for instance, exerted great influence on the implementation of the vapor extraction scheme.

This treatability study demonstrates the success of vapor extraction with an elevated mass removal with continued operation of a single well, considering a 9-month pilot test phase, in operation since May 2001. Over 45% of the infiltrated mass of contaminants was removed during this first phase. A full-scale SVE system is being implemented (2002), considering the results of pilot test operations and model sensitivity analysis.

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