

NON-ISOTHERMAL MODELING OF SOIL VAPOR EXTRACTION SYSTEM INCLUDING SOIL TEMPERATURE EFFECT

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ABSTRACT

Soil vapor extraction (SVE) is a proven effective in-situ technology for the removal of volatile organic compounds (VOCs) from the subsurface. SVE process is highly sensitive to temperature. Studying annual soil temperature variation with depth declares that there is a considerable temperature variation in the upper few meters that may affect the overall efficiency of SVE process.

A numerical model was developed to aid in investigation of field-scale soil vapor extraction process. The model is three-dimensional, time dependent that simulates nonisothermal vapor flow and transport of multicomponent mixtures in soil and keeps track of the distribution of each compound in the other three immobile phases (NAPL, aqueous, and sorbed). Rate limited interphase mass transfer with linear driving force expressions were used to model volatilization of oil into gas phase. A local equilibrium partitioning was assumed between gas, water, and solid phase. The model equations were discretized using a standard Galerkin finite element method and solved using set iterative solution algorithm.

Simulation of hypothetical field-scale problems was done. The physical domain described a three-dimensional system with flow to a single extraction well. A hypothetical soil temperature variation with depth was incorporated with the model. The result of these simulations showed that this temperature variation has a considerable effect on system efficiency and may play a role in optimum system configuration.

خلاصة

تعتبر عملية استخلاص بخار التربة تكنولوجيا موضعية مثبتة الكفاءة لازالة المركبات العضوية المتطايرة من المنطقة غير المشبعة من التربة. ان هذه العملية حساسة جدا لدرجة الحرارة. من دراسة التغير السنوي لدرجة حرارة التربة مع العمق تبين بأن هنالك تغير حراري لا بأس به في الأمتار القليلة العليا من التربة والذي من الممكن أن يؤثر على الكفاءة الكلية لهذه العملية. تم تطوير نموذج عددي للمساعدة في دراسة عملية استخلاص بخار التربة وضمن الأبعاد الحقلية. وهو نموذج ثلاثي الأبعاد و معتمد على الزمن والذي يحاكي الجريان و الانتقال متغير الحرارة لأبخرة مخلوطات المكونات المتعددة في التربة مع متابعة توزيع كل مكون في الاطوار الثلاثة الأخرى غير المتحركة (الزيتي والمائي و الممتص). تم استعمال نموذج انتقال الكتلة بين طورين ذو المعدل المحدود مع تعبير خطي للقوة الدافعة لنمذجة تطاير الزيت الى الطور الغازي مع افتراض اتزان موقعي لتوزيع الملوث بين الاطوار الثلاثة الغازي والمائي والصلب. حلت معادلات النموذج عدديا وبثلاثة ابعاد باستعمال طريقة العناصر المحدودة التقليدية standard Galerkin finite element method و باستعمال خوارزمية set-iterative. تمت محاكاة عمليات استخلاص بخار التربة بابعاد حقلية يصف المدى الفيزيائي فيها منظومة ثلاثية الأبعاد ووجود جريان بأنتاجه بئر سحب واحد. تم ادماج تغير حراري افتراضي للتربة مع النموذج العددي. أظهرت نتائج المحاكات التأثير المهم للتغير الحراري للتربة على كفاءة المنظومة وبينت انها قد تلعب دورا في تحديد الشكل الأمثل والأبعاد المثلى للمنظومة.

KEYWORDS

SVE; NAPL; soil vapor extraction; modeling; soil temperature; unsaturated zone

INTRODUCTION

Soil vapor extraction (SVE) has become the most common innovative technology for treating subsurface soils contaminated with volatile and semivolatile organic compounds. This technology employs vadose zone wells and pumps to generate gas flow through the unsaturated zone. SVE systems emphasize removal by contaminant volatilization and above ground recovery. The popularity of SVE is due in part to the low cost of vapor extraction relative to other available technologies. Vapor extraction systems are also attractive because mitigation is completed in situ. This reduces the exposure of chemical contaminants to on-site worker and off-site public. Vapor extraction offers considerable flexibility in terms of installation and operation (Hunt & Massmann, 2000).

Success of soil venting is dependent upon several site-specific factors, including the mass of spill, the type of contaminant, geohydrologic factors, and regulatory requirements regarding both site closure levels and air emission limits (Depaoli et al., 1996). In presence of oil phase, contaminant volatility will be governed by its vapor pressure and mole fraction within immiscible fluid. The vapor pressure of all compounds increases substantially with an increase in temperature. This suggests that soil temperature should be taken into account when evaluating recovery of contaminant located near the soil surface (DiGiulio, 1992).

Currently few soil extraction or bioventing models incorporate non-isothermal effects when considering system performance (Glascoe et al., 1999). Studying annual soil temperature variation with time and depth declare that there is a considerable nonlinear temperature variation with depth. Williams & Gold (1976) show that the annual range (difference between maximum and minimum about annual mean) of ground temperatures at Ottawa-Canada varies from 20°C at 0.3m depth to about 2°C at 5m depth. Similar observations for soil temperature at Griffith-Australia were presented by Marshall & Holms (1988). According to Williams & Gold (1976); Hillel (1982); Marshall & Holms (1988), for ground has constant thermal properties, the annual variation of daily average soil temperature at different depths is described with a sinusoidal function whose amplitude is decrease exponentially with distance from the surface.

A variety of methods have been used to control gas flow in the vadose zone in order to remove volatile organic compounds. Several studies recognized the effects of well configuration and engineered surface seals on gas flow and analyzed the consequence effects on the design of a vapor extraction well. These studies assumed a steady and homogeneous vadose zone temperature.

The previous studies simulate unheated SVE system with isothermal mathematical models. The effect of soil temperature variation with depth on SVE system efficiency has not been investigated. This work aims to investigate the above effect using a non-isothermal model.

Mathematical Model

This study is concerned with the non-isothermal multicomponent gas flow in the water-unsaturated soil zone and with the interfacial mass transfer of the organic contaminants between gas phase, the water phase solid phase, and the pure NAPL phase. The infiltration events are neglected and the water phase is assumed to be immobile in time, water evaporation may occur. Furthermore, the gas phase is assumed compressible, while the water phase and the soil matrix are considered incompressible. Biodegradation processes are not considered (Rathfelder et al., 1991, Hoeg et al., 2004).

The NAPL is considered to be a mixture of three volatile components (i.e. $N_o = 3$). The gas phase is modeled with composition of dry air, water vapor, and volatile constituents of the NAPL (i.e. $N_a = 5$). The aqueous phase is assumed to be comprised of water, and soluble constituents of the NAPL (i.e. $N_w = 4$). Sorption to the solid phase is restricted to components of the NAPL (i.e. $N_s=3$)

Since the quantity of contaminant dissolved in water phase and adsorbed to the solid phase is small relative to the quantity of contaminant that exists as oil phase, this study will focus on the oil phase volatilization. Equilibrium phase partitioning between gas, water, and solid phase is assumed.

Based on work presented by Rathfelder et al. (1991); Glasco et al. (1999); Adenkan et al. (1993); and Yoon et al. (2003), the following model is developed:

Flow Model Equation

$$\frac{\partial}{\partial t} \left[\frac{n S_a M_a P}{R T} \right] = \nabla \cdot \left[\left(\frac{M_a P}{R T} \right) * \left(\frac{k k_{ra}}{\mu_a} \right) \nabla P \right] + n S_a \Gamma_a \tag{1}$$

where t is time (T); n is dimensionless soil porosity; S_a is the dimensionless gas phase saturation; M_a is gas phase molecular weight (M/mole); P is gas phase pressure (ML⁻¹T⁻²); R is universal gas constant (L²θ⁻¹T⁻²/mole); T is temperature (θ); k is intrinsic soil permeability tensor (L²); k_{ra} is dimensionless relative air permeability; μ_a is gas phase viscosity (ML⁻¹T⁻¹); Γ_a is gas phase source/sink (ML⁻³T⁻¹).

Mass Transport Model Equations

Volatile Components: (γ = 1, 2, and 3)

$$\frac{\partial}{\partial t} (n S_a \rho_{a\gamma} + n S_w \rho_{w\gamma} + \rho_s \rho_{s\gamma}) = \nabla \cdot \left(\rho_{a\gamma} \frac{k k_{ra}}{\mu_a} \nabla P + n S_a D_{a\gamma}^h \nabla \rho_{a\gamma} \right) - \lambda_{ao}^{\gamma} (\rho_{a\gamma} - K_{ao}^{\gamma} \rho_{o\gamma}) \tag{2}$$

$$\frac{\partial}{\partial t} (n S_o \rho_{o\gamma}) = \lambda_{ao}^{\gamma} (\rho_{a\gamma} - K_{ao}^{\gamma} \rho_{o\gamma}) \tag{3}$$

where ρ_{aγ} is the mass concentration of γ - component in gas phase (ML⁻³); S_w is the dimensionless water saturation; ρ_s is soil bulk density (ML⁻³); ρ_{sγ} is solid phase mass concentration of γ -component (MM-1); D_{aγ}^h is the gas phase dispersion tensor of γ -component (L²T⁻¹); λ_{ao}^γ is NAPL-gas lumped mass transfer coefficient of component γ (T⁻¹); K_{ao}^γ ρ_{oγ} is the air-phase equilibrium with oil phase (ML⁻³); S_o is the dimensionless oil phase saturation; ρ_{oγ} is the mass concentration of γ - component in oil phase.

Water

$$\frac{\partial}{\partial t} (n S_a \rho_{aw} + n S_w \rho_{ww}) = \nabla \cdot \left(\rho_{aw} \frac{k k_{ra}}{\mu_a} \nabla P + n S_a D_{aw}^h \nabla \rho_{aw} \right) \tag{4}$$

where ρ_{aw} is the mass concentration of water vapor in gas phase (ML⁻³); D_{aw}^h is the gas phase dispersion tensor of water vapor (L²T⁻¹); ρ_{ww} is the mass concentration of pure water in water phase (ML⁻³).

NAPL Saturation (S_o)

$$\frac{\partial}{\partial t} (n S_o) = (\lambda_{ao}^1/\rho_1) (\rho_{a1} - K_{ao}^1 \rho_{o1}) + (\lambda_{ao}^2/\rho_2) (\rho_{a2} - K_{ao}^2 \rho_{o2}) + (\lambda_{ao}^3/\rho_3) (\rho_{a3} - K_{ao}^3 \rho_{o3}) \tag{5}$$

where ρ₁, ρ₂, and ρ₃ are the γ - component density as a pure compound (ML⁻³).

Energy Transport Model Equation :

$$\frac{\partial}{\partial t} [(n S_a \rho_a C_a + n S_o \rho_o C_o + n S_w \rho_w C_w + (1-n)\rho_s C_s)T - h_{lat,n} n S_o \rho_o - h_{lat,w} n S_w \rho_w] = \nabla \cdot (\rho_a C_a T \frac{k k_{ra}}{\mu_a} \nabla p + k_{t,eff} \nabla T) \quad (6)$$

where C_α is the specific heat capacity of phase α ($L^2 T^{-2} \theta^{-1}$); $h_{lat,n}$ and $h_{lat,w}$ are the latent heat of vaporization of NAPL and water respectively ($L^2 T^{-2}$); $k_{t,eff}$ is the volume average thermal conductivity of the soil-oil-water-gas system ($MLT^{-3} \theta^{-1}$). For partially saturated porous media an appropriate estimate of the volume average thermal conductivity is obtained from an empirical relation (Glasco et al., 1999):

$$k_{t,eff} (W m^{-1} K^{-1}) = 1.27 - 2.25n + 0.39 k_{t,s} S_w \quad (7)$$

where the $k_{t,s}$ is the thermal conductivity of the soil granular media ($k_{t,s} = 4.45 W m^{-1} K^{-1}$, typical value for sand).

Equilibrium Partition Relationships

Supplementary equilibrium partitioning relationships are needed to relate the phase concentration. The air-oil equilibrium relationships are evaluated from Raoult's Law together with Ideal Gas Law.

$$K_{ao}^\gamma = \rho_{a\gamma} / \rho_{o\gamma} = P_v^\gamma / RT \sum_{\gamma=1}^{N_o} (\rho_{o\gamma} / M_\gamma) \quad (8)$$

where

P_v^γ is γ -component vapor pressure at point temperature ($M L^{-1} T^{-2}$); M_γ is γ -component molecular weight (M/mole).

The air-water equilibrium relationships for contaminants are evaluated from Henry's Law and Ideal Gas Law.

$$K_{aw}^\gamma = \rho_{a\gamma} / \rho_{w\gamma} = M_\gamma K_h^\gamma / RT \quad (9)$$

where

K_h^γ is γ -component Henry's Law constant ($L^2 T^{-2}$).

The air-water equilibrium relationship for water vapor is evaluated from Raoult's Law together with Ideal Gas Law:

$$K_{aw}^w = \rho_{aw} / \rho_{ww} = P_v^w / RT \sum_{\gamma=1}^{N_w} (\rho_{w\gamma} / M_\gamma) \quad (10)$$

P_v^w = water vapor pressure at point temperature ($M L^{-1} T^{-2}$).

The solid-water equilibrium relationships are evaluated from equilibrium sorption partition coefficient of soil. The basis for this coefficient is the Freundlich isotherm. The lower concentration region of the Freundlich isotherm is nearly linear; that is, the mass of contaminant sorbed is directly proportional to its mass in aqueous phase. Because soil organic matter is the most common sorbent in soil, the estimation of this coefficient may be based on organic carbon content of the soil (Watts, 1997):

$$K_{sw}^\gamma = \rho_{s\gamma} / \rho_{w\gamma} = K_{oc} f_{oc} \quad (11)$$

where

f_{oc} = the dimensionless organic carbon content of the soil; K_{oc} is the organic-carbon-normalized partition coefficient ($L^3 M^{-1}$).

Numerous methods have been proposed to estimate K_{oc} (watts, 1997). Karickhoff et al. (1979) correlated K_{oc} with the contaminant water solubility for ten organic compounds, mostly aromatic:

$$\text{Log } K_{oc}(\text{ml/g}) = - .54 \text{ Log } S + .44 \quad (12)$$

where the γ -component water solubility S is expressed in mole fraction. The approach outlined is strictly useful only if f_{oc} is well above .1% (Karickhoff et al., 1979), and sorption can be assumed to be at equilibrium.

Totality Conditions

By definition fluid phase saturations sum to unity:

$$S_a + S_o + S_w = 1 \quad (13)$$

For the incompressible liquid phase at constant temperature, the component volumetric fractions sum to unity, for oil:

$$\sum_{\gamma=1}^{N_o} (\rho_{o\gamma}/\rho_o) = 1 \quad (14)$$

and for water:

$$\rho_{ww}/\rho_w + \sum_{\gamma=1}^{N_o} (\rho_{w\gamma}/\rho_w) = 1 \quad (15)$$

The gas components concentration sum to the gas phase density which is evaluated by the ideal Gas Law:

$$\rho_{aa} + \rho_{aw} + \sum_{\gamma=1}^{N_o} \rho_{a\gamma} = P M_a/RT \quad (16)$$

where ρ_{aa} and ρ_{aw} are the dry air and water vapor components, respectively (ML^{-3}).

Numerical Solution Scheme

After the flow and transport equations (1, 2, 3, 4, 5, and 6) have been discretized in three space dimensions using a standard finite element approach (Huyakorn & Pinder, 1983). The coupled nonlinear equation are solved using a modular, set-iterative solution algorithm. In this approach, the sets of flow, mass transport and energy transport are decoupled and solved separately. The set-iterative approach substantially reduces the size of solution matrices (Reeves & Abiriola, 1994). With this scheme, different grid and time discretization schemes, can potentially be applied for each equation set. The details of the numerics and model verification are described by Talib (2006).

Effect of Soil Temperature Variation on the Behavior of SVE Process in Representative Field Settings:

The finite-element model developed in this study was applied to hypothetical field-scale problem in order to demonstrate the effect of soil temperature variation on the behavior of soil vapor extraction

process in representative field settings. Three field cases shown in table 1 were simulated. Contaminants selected for this simulation were benzene, toluene and trichloroethylene.

The physical domain, shown in Fig. 1, describes a three-dimensional system with flow to a single extraction well, assuming axial symmetry. The problem scenario is an idealized representation of NAPL spill accident (Rathfelder et al., 1991 & 2000). To remediate the site an extraction well is positioned in the center of the cylindrical contamination zone. An impermeable cap is placed on the ground surface.

The flow equation was solved in the domain from the well screen to the radius of influence; r_{well} to r_{α} . Atmospheric conditions were specified at r_{α} , constant flux conditions were specified at r_{well} ; within the screened well casing pressure is evaluated from the known flux and along the blank well casing and below the well, no flow conditions were used. In the vertical direction no flow conditions were specified along the bottom boundary and along the impermeable cap at the ground surface. Atmospheric conditions were used beyond the radius of the impermeable cap.

The mass transport equations were solved in the domain from the well screen to a radius, r_c , where mass transport processes were considered insignificant. At this radius, contaminant vapor concentrations were taken to be zero. Contaminant transport at the well screen boundary was assumed to occur by advection.

The heat transport equations were solved in the domain from the well screen to a radius, r_c , where heat transport processes were considered insignificant. At this radius, temperature was taken to be governed by distributions shown in table 1. No temperature gradient toward well screen was assumed at the well screen boundary.

The soil properties and all initial contaminant distributions were assumed to be uniform. Based upon this composition, equilibrium partitioning relationships were used to evaluate the initial contaminant gas, water, and soil phase concentrations. Parameters used in this simulation were summarized in table 2. The physical data used in the simulations were listed in Talib (2006).

The flow and transport domains were discretized with an irregular mesh. Near the extraction well a high refined grid is required to capture the steep pressure gradients and large radial velocities in the gas phase. The pressure gradients, however, diminish rapidly from the well where larger spacings were used to reduce computational effort. Grid sensitivities were performed to insure solutions were sufficiently independent of mesh spacing and radius of influence.

Table 1: Temperature Distribution and Well Screen Interval within Contamination Zone for Simulations.

Case	Temp. distribution	Screen interval
1	$T = \text{constant} = 20 \text{ (}^{\circ}\text{C)}$	4m
2	$T = 30 - 10 \cdot Z/4$	4m
3	$T = 30 - 10 \cdot Z/4$	2m

note that the top of screen assumed to be at $z = 0$ for all cases, where z is the depth from the ground surface.

Table 2: (Rathfelder et al., 1991) Parameters Used in Simulations:

Configuration	
well radius (r_{well})	0.5m
screen interval	4.0m (case 1&2); 2m (case 3)
depth to top of screen	0.0m
radius of soil contamination (r_c)	7.0 m
radius of influence (r_{α})	40.0m

Field parameters

intrinsic permeability (darcy)	10.0
porosity (%)	37.3
bulk soil density (gm/cm ³)	1.75
soil mean grain size (d ₅₀) (cm)	0.06
organic carbon content, foc (%)	0.05
longitudinal dispersivity (cm)	10.0
transverse dispersivity (cm)	1.0*
gas extraction rate (m ³ /min)	3.7*

Initial saturations

oil saturation (%)	1.0
water saturation(%)	15.0

Initial oil phase mole fractions (%)

benzene	0.467
TCE	0.277
toluene	0.257

Δt (min.) 0.01-3.0

Note:

(*)(assumed in this study, based on literature review)

Simulation results are shown in Fig.'s 2, 3, and 4.

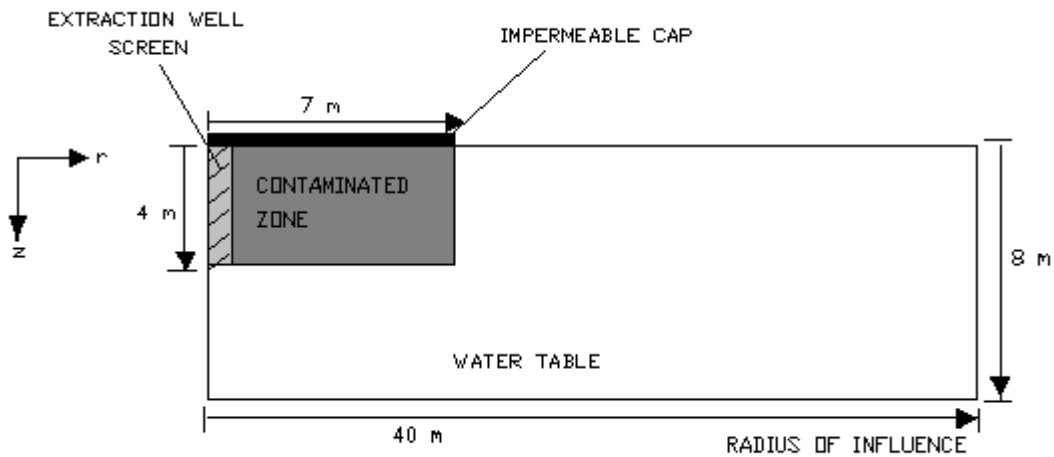


Fig. 1: Physical Domain for the Three-Dimensional Problem.

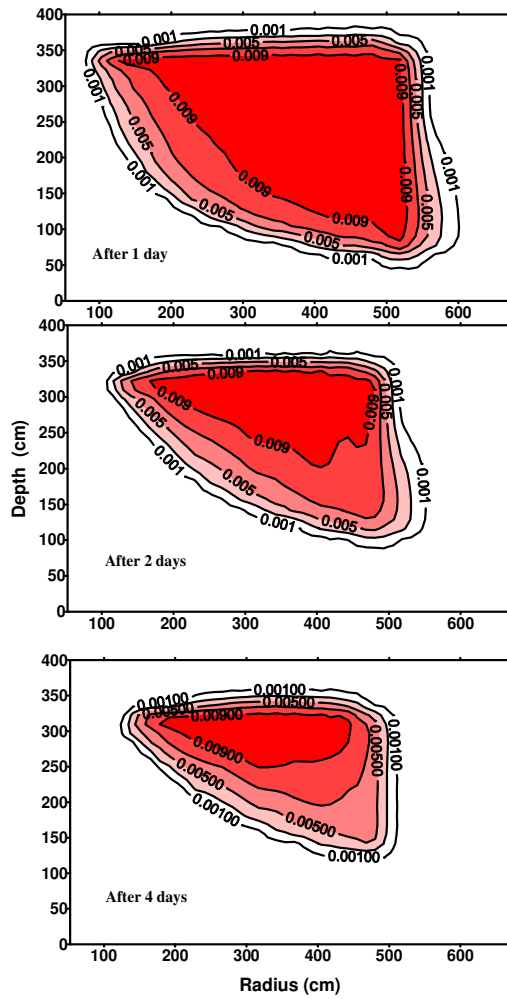


Fig. 2: Contours of Constant NAPL Saturation (S_o) Predicted from Simulation, (Case1), After 1, 2, 4 days.

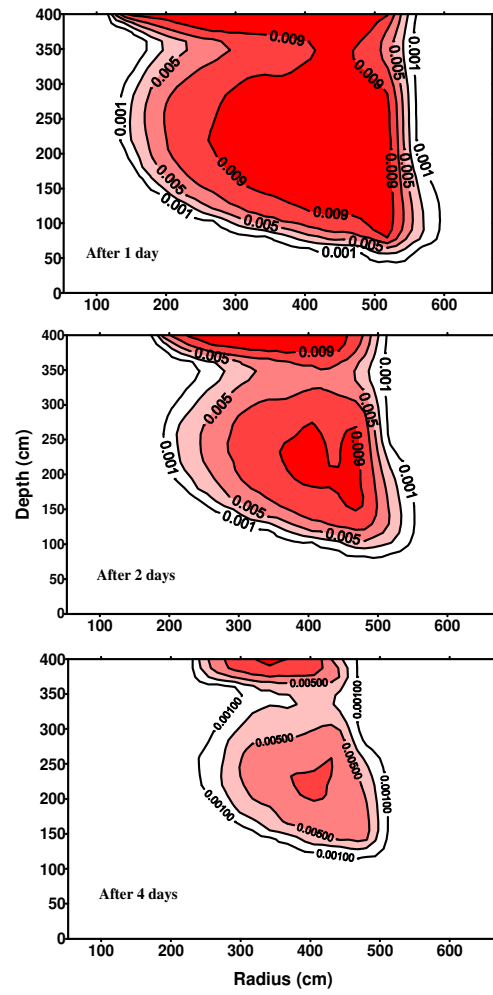


Fig. 3: Contours of Constant NAPL Saturation (S_o) Predicted from Simulation, (Case2), After 1, 2, 4 days.

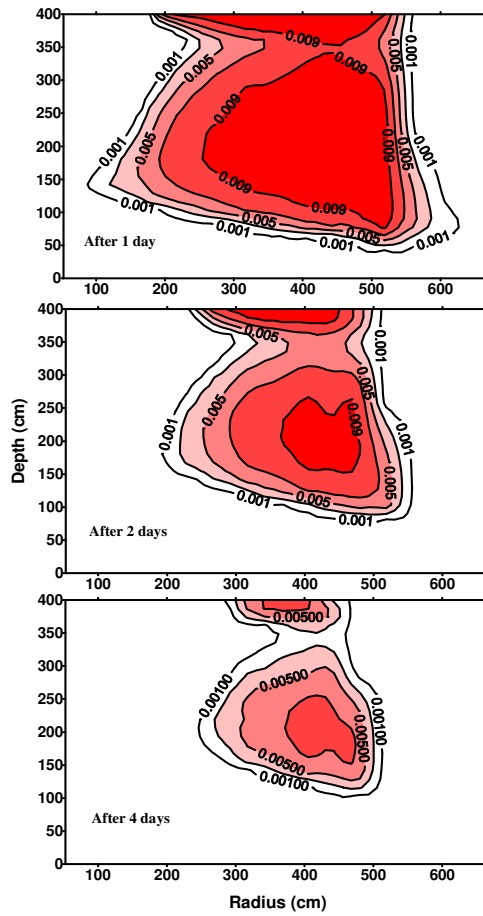


Fig. 4: Contours of Constant NAPL Saturation (S_o) Predicted from Simulation, (Case 3), After 1, 2, 4 days.

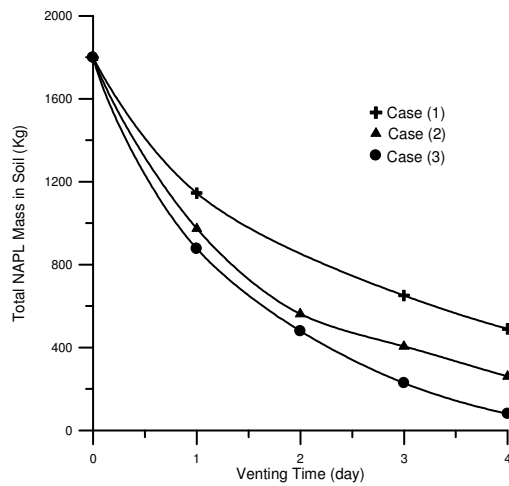


Fig.5: Predicted Total NAPL Mass Remains in Soil with Venting Time.

RESULTS AND DISCUSSION

A time series of predicted NAPL distributions in Fig.'s 2, 3 & 4 for cases 1, 2 & 3 respectively shows NAPL removal progresses radially inward. The influx of clean air along the radial and bottom horizontal boundary of the contaminated zone fastens the removal of contaminants in the early stages of venting operations. The clean air has the greatest contaminant assimilation capacity. Close to the extraction well, the increasing gas flux together with the stipulated equilibrium condition cause additional contaminant volatilization. A corresponding plot of the NAPL total mass remained in soil is shown in Fig. 5. Plots Fig.'s 2, 3 & 4 and 5 indicate that NAPL removal is greatest in the early stages of remediation. After 4 days venting, the total NAPL mass in soil is 490.1, 260.49 & 80.8 Kg for cases 1, 2 & 3 respectively.

It is clear that venting efficiency of case three is the lowest. This is evidence that the incorporation of soil temperature variation with depth in SVE numerical model for the upper few meters may predicts better venting efficiency value than the case when considering a homogenous soil temperature that exist in the deeper soil. It is clear that venting efficiency of case three is the lowest. This is evidence that the incorporation of soil temperature variation with depth in SVE numerical model for the upper few meters may predicts better venting efficiency value than the case when considering a homogenous soil temperature that exist in the deeper soil.

CONCLUSIONS

A numerical model was developed to aid in investigation of field-scale soil vapor extraction process. A hypothetical soil temperature variation with depth was incorporated with the model.

Simulation of hypothetical field-scale problems was done. Conclusions which are based on this work are summarized below:

1. Comparison of simulation results from this work with those from other researchers indicates that model advances in terms of the type and representation of processes considered leads to more complicated behavior in the simulated system dynamics, which can in turn affect interpretation of system characteristics. Shan et al. (1992); and Chen & Gosselin (1998) showed that in general, it is advantageous to screen the well close to the lower impermeable boundary because the area cleaned by the well is larger than it would be if the well was screened near the ground surface. In contrast, simulation results in this work indicate that taking soil temperature variation with depth revealed that it is advantageous to screen the well close to the hottest region. Simulation of hypothetical field-scale problems give evidence that that the lower the clean-up time may occur when the air is directed to the point of highest temperature in the multi-component contaminated zone.
2. Simulation of hypothetical field-scale problems demonstrated efficiency of venting operation is highly sensitive to soil temperature variation with depth. They give evidence that the incorporation of soil temperature variation with depth in SVE numerical model for the upper few meters may predicts better venting efficiency value than the case when considering a homogenous soil temperature that exists in the deeper soil.

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NOTATION

<u>Symbol</u>	<u>Definition</u>
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C_{α}	specific heat capacity of phase α
D_{ay}^h	the gas phase dispersion tensor
f_{oc}	dimensionless organic carbon content of the soil
$h_{lat,n}$	latent heat of vaporization of NAPL
$h_{lat,w}$	latent heat of vaporization of water
k	permeability of the soil tensor
k_{ra}	dimensionless relative air permeability
$k_{t,eff}$	volume average thermal conductivity of the soil -oil-water-gas system
$K_{ao}^{\gamma} \rho_{oy}$	air-phase equilibrium with oil phase
K_h^{γ}	γ - component Henry's Law constant
K_{oc}	organic-carbon-normalized partition coefficient
M_a	gas molecular weight
M_{γ}	γ -component molecular weight
n	dimensionless porosity
N_{α}	number of representative components comprising α - phase ($\alpha = a$ (air); o (oil); w (water); s (solid))
P	gas pressure
P_v^{γ}	γ -component vapor pressure at point temperature
P_v^w	water vapor pressure at point temperature
r_w	well radius
R	universal gas constant
S	γ -component water solubility
S_a	gas saturation
S_o	dimensionless volumetric NAPL saturation
S_w	dimensionless volumetric water saturation
S_{α}	dimensionless fluid saturation
t	time
T	temperature
z	depth below the surface



α	thermal diffusivity
Γ_a	gas phase source /sink
λ_{ao}	air-oil mass transfer factor
μ_a	gas phase viscosity
ρ_a	gas phase density
ρ_{aa}	dry air component concentration in gas phase
ρ_{aw}	water vapor component concentration in gas phase
ρ_s	bulk soil density
ρ_{sy}	solid phase mass concentration of γ -component
ρ_w	water density
ρ_{ww}	pure water component concentration in water phase
ρ_α	mass density of α -fluid
$\rho_{\alpha\gamma}$	mass concentration of γ -component in the α - phase
ρ_γ	γ -component density as a pure compound

ABBREVIATIONS:

NAPL	Non-Aqueous Phase Liquid
SVE	Soil Vapor Extraction
TCE	TriChloroEthylene
VOC	Volatile Organic Compound