

## NUMERICAL MODEL OF THE MIGRATION OF TOLUENE IN POROUS MEDIA

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**Abstract:** A Volatile Organic Compound (VOC) model describing migration of toluene concentration in subsurface system of porous media was developed. To investigate pollutant transport of nonaqueous phase liquids (NAPL) for VOC, requires a solution of multiphase fluid flow, heat flow and pollutant transport in a deforming porous media. The nonlinear saturation and relative permeability functions were incorporated into Galerkin finite element model, which was subsequently used to simulate multiphase immiscible fluid flow under unsaturated conditions. The governing partial differential equations, in terms of soil displacements, fluid pressures, concentrations and temperature, which are coupled and non-linear, are solved by the finite element method. The weighted residual finite element approach was employed to achieve spatial discretization of the problem while temporal discretization was achieved by a fully implicit scheme. The potential use of the numerical model is discussed and applied to toluene migration in one-dimensional analysis to demonstrate the model capabilities.

**Keywords:** *Groundwater; Unsaturated Zone; Finite Element; Toluene; Multiphase Flow; Heat and Volatilisation.*

**Abstrak:** Satu model Bahan Organik Meruap (VOC) telah dibangunkan untuk menggambarkan pergerakan kepekatan toluene bagi sistem sub-permukaan dalam media berliang. Pergerakan pencemar oleh fasa cecair tidak berair (NAPL) seperti VOC memerlukan satu penyelesaian dalam aliran bendalir berbilang fasa, aliran haba dan pergerakan bahan pencemar dalam mengubah bentuk bahantara berliang. Fungsi ketepuan tidak lurus dan kebolehtelapan nisbi telah digabungkan di dalam model Galerkin elemen tak terhingga yang kemudiannya digunakan untuk simulasi aliran bendalir tidak bercampur berbilang fasa di bawah keadaan tidak tepu bagi bahantara berliang tersebut. Pembentukan persamaan pembezaan separa seperti anjakan tanah, tekanan bendalir, kepekatan dan suhu yang saling bergandingan dan tidak lurus telah diselesaikan dengan menggunakan kaedah elemen tak terhingga. Pendekatan *weighted residual* dalam elemen tak terhingga diambil untuk menyusun atur ruang manakala susun atur sementara pula adalah menggunakan kaedah mutlak (implicit) sepenuhnya. Potensi kegunaan kaedah berangka ini dibincangkan dengan contoh bagi pergerakan toluene dalam analisis satu dimensi untuk membuktikan keupayaan model.

**Katakunci:** *Airbumi; Zon Tak Tepu; Elemen Tak Terhingga; Toluene; Aliran Berbilang Fasa; Haba dan Pemeruapan.*

## 1. Introduction

Groundwater contamination has become a major issue since the exposure of numerous hazardous waste sites in the late seventies. The migration of contaminants, process of dissolution, factors of influence, effects and the techniques for remediation of groundwater contamination are the main area of research to ensure sustainable use of groundwater resources. Due to these, research techniques are needed in order to simulate the behaviour of groundwater contamination. An understanding of the mechanisms of pollutant transport is very important in predicting Volatile Organic Compound (VOC) volatilisation from the soil system. Many highly toxic contaminants commonly found in the subsurface occur as slightly soluble and highly volatile fluids and immiscible with water. Despite of their low solubility, these compounds post a widespread potential threat to the groundwater resources. The important characteristics of the contaminant to be considered include vapour pressure, aqueous solubility, Henry's law constant, diffusion coefficient and the ability of contaminants to degrade. Organic compounds have a potential to degrade biologically and chemically. Thus, contaminants with high vapour pressure will volatilise more quickly compared to contaminants with lower vapour pressures such as pesticide. However, the major contaminant property affecting volatilisation is its vapour pressure while the factors affecting contaminant mobility are various air or water partition coefficients, of the soil system. Numerical model is one of the techniques that has been developed to quantify and describe groundwater contamination phenomena. In addition, laboratory works and field studies have been carried out in order to understand the processes of contamination as well as to get data required in model verification. Most of the experiments and models were developed to assess the impact of contaminant concentration on the subsurface systems, especially for petroleum by-products. Accordingly, these types of contaminants had been recognized for a long time compared to other types of chemical contaminants.

In unsaturated soil, organic compounds may dissolve into the water phase and volatilise into the gas phase. The indicator parameter to measure the ability of the organic compound to dissolve in water is called the water solubility. Upon dissolving into the aqueous phase, the solute is then transported to the saturated zone. High infiltration rate and a greater mass of high water soluble compounds could be leached into the aqueous phase compared to fractions that diffused in the gas phase (Muhammad Nassir, 1991). In reality, contaminant transport in the unsaturated zone is much more complex than in the saturated zone mainly because of numerous phases involved, i.e. soil, water, air and contaminant. Chemicals exist in the unsaturated zone in four phases: dissolved in soil moisture, sorbed to the soil particles, as nonaqueous phase liquids (NAPL) and as an enveloped of organic vapours. These organic vapours have been identified as the more ubiquitous groups of hazardous chemicals present in contaminated soils and groundwater. They can migrate much faster than the liquid phase. Moreover, the vapour flow velocities and direction are not controlled by groundwater gradients.

## 2. Physical Model Properties and Consideration

An unsaturated soil has more than two phases and the pore water pressure is negative relative to the pore air pressure. Negative pressure is defined as the capillary pressure, which exists only for a fluid pressure less than zero. In unsaturated zone, the pore water pressure is negative under static equilibrium conditions with respect to the water table. The negative pore water pressure head has a linear distribution with depth. Thus, in any soil, that is near the ground surface and present in a relatively dry environment is subjected to negative pore water pressures and possible desaturation (Fredlund and Rahardjo, 1993).

The physical model for multiphase flow within an unsaturated flow regime can be described as follows:

- a) The phase saturation value sum to unity, i.e.:

$$S_n + S_w + S_g = 1 \tag{1}$$

where  $S_n$  is the NAPL saturation,  $S_w$  is the water saturation and  $S_g$  is the gas saturation.

- b) Capillary pressure and temperature are function of saturation, i.e.;

$$S_\alpha = f(P_{c\alpha w}, P_{cnw}, T) \tag{2}$$

where,  $P_{c\alpha w} = P_g - P_w$  and  $P_{cnw} = P_n - P_w$ . These equations are function of two capillary pressure values (gas, water, NAPL and temperature).

The nonisothermal case refers to conditions where temperature is not a constant.

- c) Relative permeability is a function of saturation, i.e.;

$$K_{rw} = K_{rw}(S_w) \tag{3a}$$

$$K_{rn} = K_{rn}(S_w, S_g) \tag{3b}$$

$$K_{rg} = K_{rg}(S_g) \tag{3c}$$

- d) The pressures are function of density and viscosity.

The distribution of the zones as a function of capillary pressure and the relative permeabilities for water,  $k_{rw}$ , and gas,  $k_{rg}$  phases are calculated from capillary pressure values using the equations by Brooks and Corey (1964) and the relative permeability for NAPL,  $k_{rn}$  based on Lujan (1985) as below:

$$k_{rg} = S_{we}^{\frac{(2+3\lambda)}{\lambda}} \tag{4a}$$

$$k_{rg} = (1 - S_{te})^2 \left(1 - S_{te} \frac{(2+\lambda)}{\lambda}\right) \tag{4b}$$

$$k_{rn} = (S_{te} - S_{we})^2 \left(S_{te} \frac{(2+\lambda)}{\lambda} - S_{we} \frac{(2+\lambda)}{\lambda}\right) \tag{4c}$$

which,

$$S_{we} = \left(\frac{S_w - S_{rw}}{S_{max}}\right), \quad S_{te} = \left(\frac{1 - S_g - S_{rw} - S_{rn}}{S_{max}}\right)$$

Where  $S_{we}$  is the effective water saturation and  $S_{te}$  is the total effective liquid saturation. In the fluid density function, for a non-isothermal case, the thermal effects on the rate of fluid accumulation in the mass conservation equation are also considered. The solid density  $\rho_s$  and the pore liquid density  $\rho_a$  are assumed to be pressure, temperature and contaminant concentration dependent (Norhan and Lewis, 1997) as below:

$$\rho_w = \rho_w(P_w, T, C_w) \tag{5a}$$

$$\rho_g = \rho_g(P_g, T, C_g) \tag{5b}$$

$$\rho_n = \rho_n(P, T) \tag{5c}$$

$$\rho_s = \rho_s(P, T) \tag{5d}$$

The fluid density is taken to be a linear function of pressure, temperature and contaminant concentration. For flow solubility the organic contaminants also require a consideration of the interphase mass transfer. Dissolution and volatilization of the NAPL phase are responsible for the input of the pollutant into the groundwater and soil gas, and gas water partitioning can significantly affect transport within these phases (Dorgaten and Tsang, 1992).

The dissolution rate is controlled by  $C_{wm}$  which is the equilibrium concentration of the organic matter in the water phase and controlled by a rate coefficient,  $\kappa_{nw}$  where:

$$\frac{\partial C_g}{\partial t} = \kappa_{ng} (C_{gm} - C_w) \tag{6a}$$

and

$$\frac{\partial C_g}{\partial t} = \kappa_{wg} (HC_w - C_g) \tag{6b}$$

where  $C_{gm}$  is the equilibrium concentration in the vapour phase,  $C_g$  is the concentration of organic constituent in the gas phase, and  $\kappa_{ng}$  is the mass transfer coefficient for volatilization of organic compounds in the vapour phase. Interphase mass transfer by dissolution and volatilization will generally be the dominating phase exchange in regions where a significant amount of NAPL phase is present. Gas-water partitioning is mainly controlled by

Henry's law with a constant value of  $H$  that expresses the relation between  $C_g$  and  $C_w$  at equilibrium, where  $H = \frac{C_{gm}}{C_{wm}}$ , and  $\kappa_{wg}$  is the mass transfer coefficient for gas-liquid partitioning between the water and gas phases.

### 3. Theoretical Formulation

The molar concentration of the air is given by  $c_{gj}$  and could be derived from Dalton's law. Hence, by assuming that dry air and water vapour behave as ideal gases, the gas phase pressure is;

$$P_g = P_j + P_v + P_i \tag{7}$$

where  $P_j$ ,  $P_v$  and  $P_i$  represent the partial pressures of air, water vapour and the contaminant gas respectively. Introducing the ideal gas assumption and simplifying yields the molar concentration of dry air,  $c_{gj}$  (Thomas and Ferguson, 1998):

$$c_{gj} = \frac{P_g}{RT} - \frac{\rho_v R_v}{R} - c_{gi} \quad (\text{molm}^{-3}) \tag{8}$$

where  $\rho_v$  is vapour density and  $R_v$  is specific gas constant for water vapour. The sum of the molar concentrations,  $c_g$ , which relates to the gas phase pressure  $P_g$  (Pa) and its absolute temperature  $T$  ( $^{\circ}$ K) by the ideal gas law, now becomes:

$$\sum c_i = c_g = c_{gj} + c_{gi} = \frac{P_g}{RT} - \frac{\rho_v R_v}{R} \quad (\text{molm}^{-3}) \tag{9}$$

The equation for mass density,

$$\rho_g = \frac{M_{gj}}{1000R} \left( \frac{P_g}{T} - \rho_v R_v \right) + \frac{M_{gi} - M_{gj}}{M_{gj}} c_{gi} \tag{10}$$

Finally, the density of the gas phase becomes,

$$\left( \frac{d\rho_g}{dT} \right)_P = \frac{M_{gj} P_g}{1000RT^2} \tag{11}$$

$$\left( \frac{d\rho_g}{dP_g} \right)_T = \frac{M_{gj}}{1000RT} \tag{12}$$

$$\left( \frac{d\rho_g}{dC_{gi}} \right) = \frac{M_{gi} - M_{gi}}{M_{gi}} = \beta_{cg} \quad (13)$$

The gas and water phase tortuosity is taken from the Millington and Quirk model as :

$$\tau = \phi^{1/3} S^{7/3} \quad (14)$$

by assuming that local chemical equilibrium exists between the liquid or organic phase, gas phase and water phase. Partitioning between water and gas is common and is described by Henry's law where the Henry constant of low solubility can be calculated by a formulation governs by Jury et. al (1983) as follow:

$$H = \frac{C_i}{C_w} \quad (15)$$

where  $C_w$  is the solubility of the organic in water ,  $H$  is Henry's constant for the organic material and the parameter for  $h$  can be represented as,  $h = \frac{1}{H}$ .

### 3.1 Governing Equation

The governing equations adopted in this VOC model such as soil equation, multiphase equation and energy equation were derived from the previous work by Norhan (1998). The multiphase flow equation especially in gas phases, which consists of vapour flow and dry air equations is referred to the equation of contaminant from Thomas and Ferguson (1998).

### 3.2 Multiphase Flow Equation

In the multiphase flow equation, the fluid phase behaviour of immisible and incompressible fluids flowing in a deforming porous media can be obtained by combining Darcy's linear flow with the mass conservation balance for each of the flowing phases. Lewis and Schrefler (1987) have previously studied this behaviour of contaminant then continued by Norhan (1998) with additional processes of interphase mass transfer. The Darcy's velocity can be expressed as:

$$V = -\frac{1}{\mu} K \nabla (P + \rho g h) \tag{16}$$

where,  $K$  represents the absolute permeability matrix of the medium ( $L^2$ ),  $\mu$  is the dynamic viscosity of the fluid ( $ML^{-1}T^{-1}$ ),  $g$  is the gravitational constant ( $LT^{-2}$ ) and  $h$  is the head above a given datum.

The general form of the continuity equation for each of the phase can be expressed as:

$$\begin{aligned} & -\nabla^T \left[ \frac{K k_{ra} \rho_a}{\mu_a B_a} \nabla (P_a + \rho_a g h) \right] + \\ & \rho_a \frac{S_a}{B_a} \left[ \left( m^T - \frac{m^T D_r}{3K_s} \right) \frac{\partial \varepsilon}{\partial t} + \frac{m^T D_r C}{3K_s} + \left( \frac{(1-\phi)}{K_s} - \frac{m^T D_r m}{(3K_s)^2} \right) \frac{\partial \bar{p}}{\partial t} + \right. \\ & \left. \left( -(1-\phi)\beta_s + \frac{m^T D_r m \beta_s}{3K_s} \right) \frac{\partial T}{\partial t} \right] + \\ & \phi \frac{\partial}{\partial t} \left( \frac{\rho_a S_a}{B_a} \right) + \rho_a Q_a + \Gamma_a = 0 \end{aligned} \tag{17}$$

where,

$$\phi \frac{\partial}{\partial t} \left( \frac{\rho_a S_a}{B_a} \right) = \phi \frac{\rho_a}{B_a} \frac{\partial S_a}{\partial t} + \phi \frac{S_a}{B_a} \frac{\partial \rho_a}{\partial t} + \phi \rho_a S_a \frac{\partial}{\partial t} \left( \frac{1}{B_a} \right)$$

$$\Gamma_w = -\phi S_w \kappa_{nw} (C_{wm} - C_w) + \phi S_g \kappa_{wg} (HC_w - C_g)$$

$$\Gamma_g = -\phi S_g \kappa_{ng} (C_{gm} - C_g) + \phi S_w \kappa_{wg} (HC_w - C_g)$$

where  $\phi, \Gamma$  and  $Q$  are the porosity of the medium, internal sinks or sources due to interphase mass transfer and internal sinks or sources. Equation (17) is called a multiphase incompressible fluid flow with interphase mass transfer for an isotropic soil in deforming porous medium. Additionally, this equation is strongly coupled and nonlinear, due to the dependence of the saturations on the capillary pressures and represents the general governing equation for multiphase incompressible fluid flow with interface mass transfer for an isotropic soil. The mobility terms in this equation are also strongly dependent on the unknowns. Furthermore, the fluid flow is coupled with the transport, due to the dependence of the densities on the concentration and due to interphase mass transfer.

### 3.3 Vapour Flow Equation

The development of the equilibrium of vapour equation is based on the theoretical approach from Thomas and Ferguson (1998). The governing principle of vapour flow is as stated below:

$$\frac{\partial(P_w \theta_v)}{\partial t} = -\nabla \cdot (\rho_w V_v) - \nabla \cdot (\rho_v V_g) \quad (18)$$

and;

$$\theta_v = \frac{\phi S_g \rho_v}{\rho_w}$$

where  $\theta_v$ ,  $\rho_v$ ,  $V_v$  and  $V_g$  are the volumetric vapour content, water vapour density, vapour velocity and gas velocity, respectively. This equation assumes that the liquid water and the water vapour are in equilibrium at every instance. The value of  $S_g$  denotes the gas saturation and it is a function of temperature.

### 3.4 Dry Air Equation

At the constant temperature, the weight of gas that dissolves in a given volume of liquid is directly proportional to the pressure of the gas with which it is in contact. By invoking the principle of conservation of mass to the dry air phase yields (Thomas and Ferguson, 1998):

$$\frac{\partial}{\partial t} [\phi C_{gj} (S_g + H_{air} S_w)] = -\nabla [C_{gj} (V_g + H_{air} V_w)] \quad (19)$$

where  $H_{air}$  is Henry's coefficient for air,  $C_{gj}$  is the molar concentration of the contaminant gas,  $V_g$  and  $V_w$  are the gas velocity and water velocity and  $S_g$ ,  $S_w$  are the saturation of gas and saturation of water, respectively.

### 3.5 Gas Migration Equation

The contaminant gas migration is based on the principle of mass conservation and assumed that gas and liquid velocities of the contaminant gas are equal to those of the gas mixture gives (Thomas and Ferguson, 1989):

$$\frac{\partial}{\partial t} (\phi S_g C_{gi} + \phi H_i S_w C_{gi}) = \nabla [(D_g + H_i D_w) \nabla C_{gi}] - \nabla [(V_g + H_i V_w) C_{gi}] \quad (20)$$

where,  $D_g$ ,  $D_l$  and  $H_i$  are the effective diffusion coefficient, the hydrodynamic coefficient and Henry's law coefficient for the contaminant gas, respectively.



### 3.6 Energy Transport Equation

Referring to Norhan (1998), the energy conservation equation for nonisothermal simulation within a porous medium, is expressed as:

$$\begin{aligned} & \frac{\partial}{\partial t} [(1-\phi)\rho_s C_{ps} + \phi\rho_w S_w c_{pw} + \phi\rho_g S_g c_{pg} + \phi\rho_n S_n c_{pn}]T \\ & + \rho_w S_w c_{pw} V_w \cdot \nabla T + \rho_g S_g c_{pg} V_g \cdot \nabla T + \rho_n S_n c_{pn} V_n \cdot \nabla T = \nabla \cdot (\lambda_T \nabla T) \\ & + (1-\phi)\rho_s Q_s + \phi\rho_w S_w Q_w + \phi\rho_g S_g Q_g + \phi\rho_n S_n Q_n \end{aligned} \quad (21)$$

Where;

$$\begin{aligned} & \frac{\partial}{\partial t} [(1-\phi)\rho_s C_{ps} + \phi\rho_w S_w c_{pw} + \phi\rho_g S_g c_{pg} + \phi\rho_n S_n c_{pn}]T = \\ & [(1-\phi)\rho_s C_{ps} + \phi\rho_w S_w c_{pw} + \phi\rho_g S_g c_{pg} + \phi\rho_n S_n c_{pn}] \frac{\partial T}{\partial t} + \\ & T(1-\phi)\rho_s \frac{\partial \rho_s}{\partial t} + T\phi\rho_w c_{pw} \frac{\partial S_w}{\partial t} + T\phi S_w c_{pw} \frac{\partial \rho_w}{\partial t} + T\phi\rho_g c_{pg} \frac{\partial S_g}{\partial t} + \\ & T\phi S_g c_{pg} \frac{\partial \rho_g}{\partial t} + T\phi\rho_n c_{pn} \frac{\partial S_n}{\partial t} + T\phi S_n c_{pn} \frac{\partial \rho_n}{\partial t} \end{aligned}$$

where  $\rho c_{p\alpha}$  is the heat capacity of the liquid or soil phase,  $T$  is temperature,  $V$  is apparent velocity of the fluid and  $\lambda_T$  is the thermal conductivity matrix of the soil.

### 3.7 Initial and Boundary Conditions

The initial and boundary conditions for the nonisothermal problem must be complemented by an appropriate condition for heat flow. Thus, the initial conditions within porous media are specified as:

$$u_i = u_i^o \quad P_\alpha = P_\alpha^o \quad C_\theta = C_\theta^o \quad T = T^o$$

The boundary conditions are specified as by prescribed values,

$$u_i = \bar{u}_i \quad \text{on } \Gamma_u \quad \text{and} \quad \sigma_{ij} n_j = t_j \quad \text{on } T_i \quad \text{where } \Gamma_u \cup T_i = \Gamma$$

$$\text{and, } P_\alpha = P_\alpha^b \quad C_\theta = C_\theta^b \quad T = T^b$$

$$\text{or flux : } q_{\alpha} = -\frac{Kk_{\alpha}\rho_{\alpha}}{\mu_{\alpha}} \nabla(P_{\alpha} + \rho_{\alpha}gh)n$$

where  $b_i$  is the body force,  $t_j$  is the imposed traction,  $\bar{u}_i$  is the external displacement,  $q_x$  is the flux,  $o$  represents the initial conditions and  $n$  is the vector normal to the boundary.

#### 4. Discretization and Solution Procedure

In this solution procedure, the governing equations were carried out by finite element in space and finite difference in time. In the space discretization, the unknowns are associated with 'nodes' or 'nodal points', which were distributed in a logical manner around the perimeter of the element. A weak formulation of the governing equations could be obtained by applying Galerkin's procedure of weighted residuals. The Gauss theorem was used to transform the second spatial derivatives.

The primary unknowns such as displacements, fluid pressures, temperature and concentrations were determined by a fully coupled nonsymmetrical and highly nonlinear system of ordinary differential equation in time. In this method, an implicit scheme was used, since all the non-linear coefficients were dependent on the unknowns. The iterative procedures are usually performed within each time step to obtain the final solution.

#### 5. Numerical Analysis

This analysis showed the migration of toluene in unsaturated zone. One-dimensional simulation of toluene was performed with the same surface temperature with an initial water saturation of 0.445. The domain of soil column used was 1 m in height. The initial and boundary conditions used in the simulation are given in Table 1. The values of vapour pressure, molecular weight and Henry's law constant for toluene are 0.037 atm, 92.1 gmol<sup>-1</sup> and 0.26, respectively.

Table 1: Boundary and initial condition of model

Initial condition	Value
Water Saturation, $S_w$	0.445
Gas pressure, $P_g$	101325 Nm <sup>-2</sup>
Water pressure, $P_w$	-420 x 10 <sup>4</sup> Nm <sup>-2</sup>
Temperature, $T$	293.15 K
Boundary condition:	
Lateral Surface	$\mu_h = 0, q_w = 0, q_g = 0$
Top surface:	
• $P_w$	-280 x 10 <sup>4</sup> Nm <sup>-2</sup>
• $P_g$	101325 Nm <sup>-2</sup>
• $T$	323.15K
Bottom surface:	$\mu_v = 0, q_w = 0, q_g = 0$

This simulation was conducted with intrinsic permeability of soil,  $K = 1.0 \times 10^{-13} \text{ m}^2$  and  $1.0 \text{ mgL}^{-1}$  of concentration introduced at the top surface of soil column without initial value of concentrations. The physical properties used for the analysis were as follows,

Elastic modulus	$E = 10.0 \times 10^6 \text{ Nm}^{-2}$
Poisson ratio	$\nu = 0.3$
Porosity	$\phi = 0.5$
Gas viscosity	$\mu_n = 1.81 \times 10^{-5} \text{ Pa. S}$
Bulk modulus	$K_s = 6.1 \times 10^8 \text{ Nm}^{-2}$
Gas diffusion	$D_g = 1.0 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$
Liquid water diffusion	$D_w = 1.0 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$
Density for toluene	$\rho_n = 862.0 \text{ kgm}^{-3}$
$P_{dgw}$	$225.0 \times 10^3 \text{ Nm}^{-2}$
$k_{rg}$	$S_g^3$
$S_w$	0.10
Initial NAPL saturation	$S_n = 0.25$
Initial gas saturation	$S_g = 0.60$
$\lambda$	3.0
NDF	$U, P_w, P_g, T, C_{gi}$

Mass fraction results for toluene simulation are shown in Figure 1. Results are plotted for the depths of 0.7 m, 0.5 m and 0.3 m along time. This simulation was carried out, when  $1.0 \text{ mgL}^{-1}$  of concentration was introduced at the top boundary condition and no initial concentration was applied. Then, results shown at that, the maximum values of mass fraction at depth of 0.3 m, 0.5 m and 0.7 m were around  $36.52 \times 10^{-10}$ ,  $21.36 \times 10^{-10}$  and  $5.58 \times 10^{-10}$  respectively. These maximum values occurred at simulation time of approximately 10 hrs.

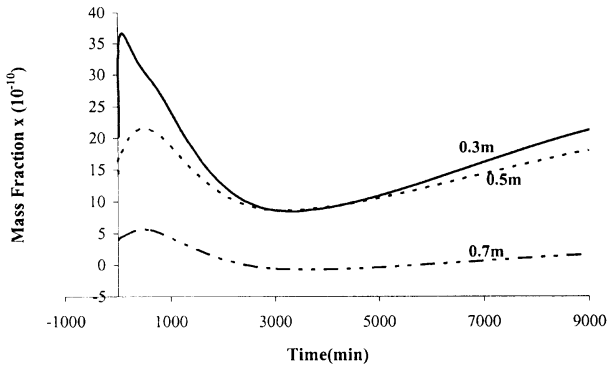


Figure 1: Distribution of toluene concentration in soil ( $K=1.0 \times 10^{-13} \text{ m}^2$ )

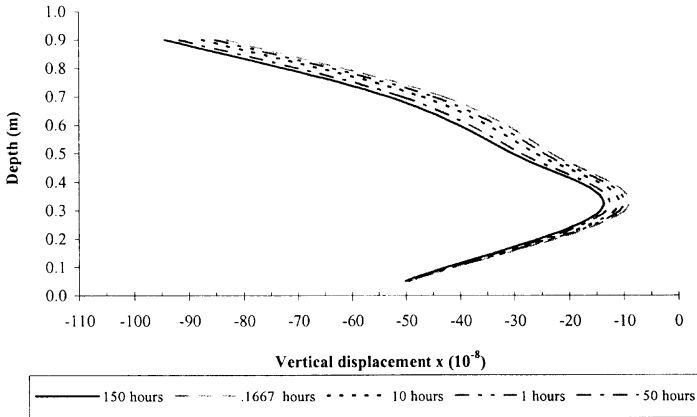


Figure 2: Vertical displacement of toluene in soil ( $K=1.0 \times 10^{-13} \text{ m}^2$ )

Vertical displacements along soil column are plotted in Figure 2. The displacement is very small throughout the soil column for 0.1667 hours, 1 hour, 10 hrs, 50 hrs and 150 hrs. Meanwhile, Figure 3 and Figures 4a to 4d show the profiles of computed gas pressure in soil and the temperature effect throughout the soil column at 1, 10, 50 and 150 hrs. For gas pressure distribution, the gas pressure increased with a small value of increment. Resulting profile of temperature effect for toluene throughout soil column for

1, 10, 50 and 150 hrs are presented in Figures 4a to 4b. Then, results illustrate that at 150 hrs, the temperature was only  $0.00070317^{\circ}\text{C}$ , showing that the variation of temperature throughout the soil column was very small.

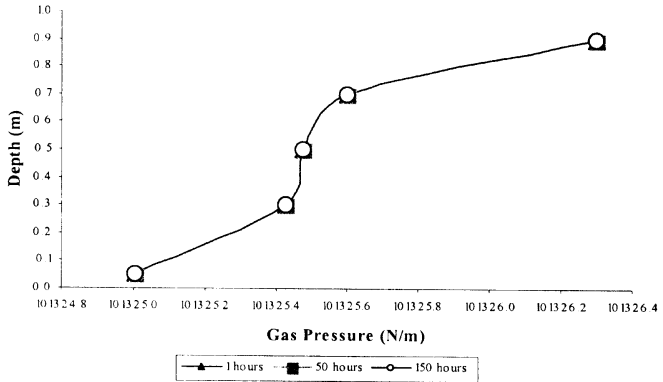


Figure 3: Gas pressure distribution with soil depth

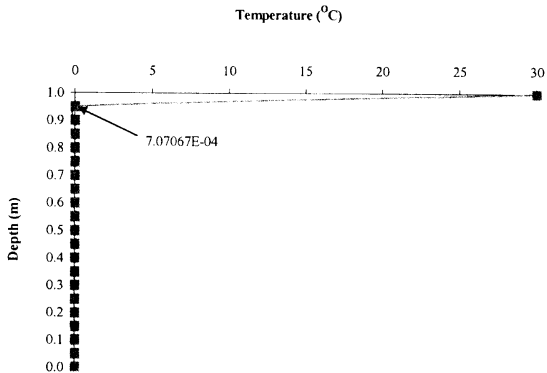


Figure 4a: Temperature profile of toluene at 1 hr

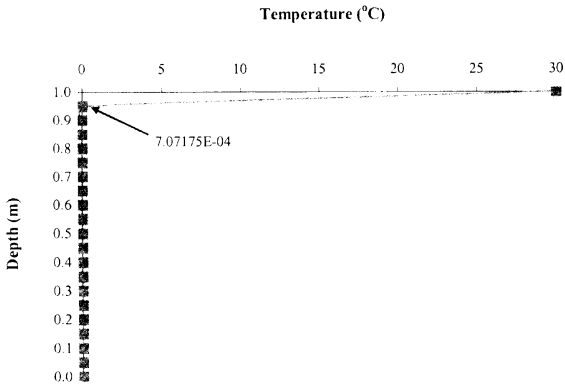


Figure 4b: Temperature profile of toluene at 10 hrs

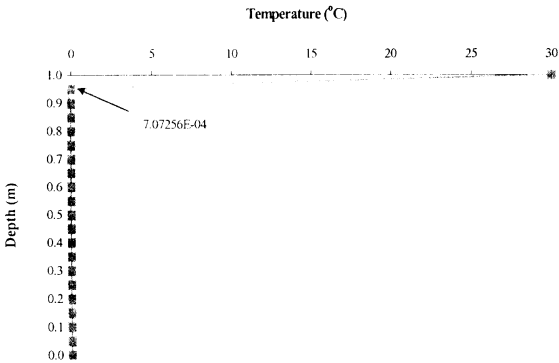


Figure 4c: Temperature profile of toluene at 50 hrs

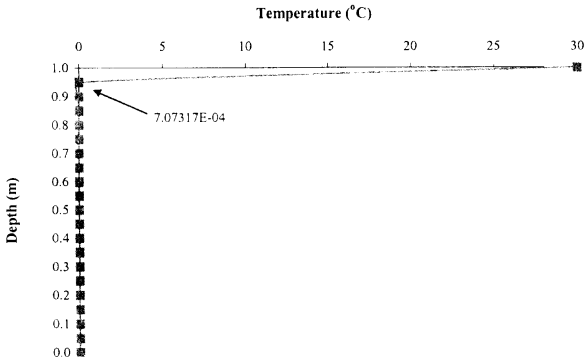


Figure 4d: Temperature profile of toluene at 150 hrs

## 7. Conclusion

The simulation results presented in this study have demonstrated that the parameters effect of VOC volatilisation for NAPL contaminant such as density advection and diffusion of contaminant, temperature and characteristics of contaminant are the dominant factors for predicting the migration of toluene in porous media. Henry's law constant is required to predict the behaviour of organic compounds in the environment to describe the movement of volatile pollutants from air to water or from water to air phase. Knowledge in Henry's law constant is very crucial in assessing the environmental risk caused by chemical movement. These factors cannot be ignored when modelling the migration of VOC transport in porous media.

A numerical model, describing the migration of contaminant gas (VOC model) through soil in a deforming porous medium under nonisothermal condition has been discussed and presented. The migration of toluene in one-dimensional analysis has been performed to demonstrate the model capability for geoenvironmental applications.

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