



Research papers

Analytical solutions for a soil vapor extraction model that incorporates gas phase dispersion and molecular diffusion

Junqi Huang^{a,*}, Mark N. Goltz^b^a Ground Water and Ecosystems Restoration Division, National Risk Management Research Laboratory, U.S. EPA, Ada, OK 74820, USA^b Department of Systems Engineering and Management, Air Force Institute of Technology, 2950 Hobson Way, WPAFB, OH 45433, USA

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ABSTRACT

To greatly simplify their solution, the equations describing radial advective/dispersive transport to an extraction well in a porous medium typically neglect molecular diffusion. While this simplification is appropriate to simulate transport in the saturated zone, it can result in significant errors when modeling gas phase transport in the vadose zone, as might be applied when simulating a soil vapor extraction (SVE) system to remediate vadose zone contamination. A new analytical solution for the equations describing radial gas phase transport of a sorbing contaminant to an extraction well is presented. The equations model advection, dispersion (including both mechanical dispersion and molecular diffusion), and rate-limited mass transfer of dissolved, separate phase, and sorbed contaminants into the gas phase. The model equations are analytically solved by using the Laplace transform with respect to time. The solutions are represented by confluent hypergeometric functions in the Laplace domain. The Laplace domain solutions are then evaluated using a numerical Laplace inversion algorithm. The solutions can be used to simulate the spatial distribution and the temporal evolution of contaminant concentrations during operation of a soil vapor extraction well. Results of model simulations show that the effect of gas phase molecular diffusion upon concentrations at the extraction well is relatively small, although the effect upon the distribution of concentrations in space is significant. This study provides a tool that can be useful in designing SVE remediation strategies, as well as verifying numerical models used to simulate SVE system performance.

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1. Introduction

Soil vapor extraction (SVE) is a physical treatment process for in situ remediation of volatile organic contaminants (VOCs) in the vadose zone. The process involves inducing air flow in unsaturated soil, thereby enhancing the in situ volatilization of the VOC from dissolved and separate (i.e., non-aqueous phase liquid (NAPL)) phases, accompanied by transfer of the contaminants from the sorbed phase into the gas phase. The gas containing the contaminants is then pumped out via an extraction well. The engineering performance of an SVE system is governed by the processes affecting VOC fate and transport (e.g., advection, dispersion, inter-phase mass transfer and decay) (Gierke et al., 1992; Travis and Macinnis, 1992; Cho et al., 1993; Armstrong et al., 1994; Popovicova and Brusseau, 1998; Lorden et al., 1998). Conventionally, SVE models simulate VOC transport in a convergent gas flow

field (e.g., Goltz and Oxley, 1994). Because of the dependence of the gas flow velocity on radial distance, the dispersion coefficient (D) is also modeled as a function of radial distance, and may be represented as $D = a_L v(r) + D_m$, where a_L is the longitudinal dispersivity, $v(r)$ is the velocity of gas flow as a function of the radial distance (r), and D_m is the effective molecular diffusion coefficient in the vadose zone. To analytically solve the radial advective/dispersive transport equation, some simplifications are usually implemented. In particular, a number of models have been presented to describe transport in both the saturated and unsaturated zone that neglect molecular diffusion ($D_m \equiv 0$) (Chen, 1985, 1987; Moench, 1989, 1995; Chen et al., 2002, 2003; Huang et al., 2010; Wang and Zhan, 2013; Goltz and Oxley, 1991; Goltz and Oxley, 1994; Huang and Goltz, 1999; Lai et al., 2016). Chen et al. (2007) developed an approximate analytical model that incorporated both dispersion and molecular diffusion to simulate SVE. The Chen et al. (2007) model approximated the exact solution by linearly coupling and weighting the diffusion- and dispersion-dominated analytical solutions, using a composite parameter (a Peclet number that characterized the combination of diffusive and dispersive processes).

* Corresponding author.

E-mail addresses: huang.junqi@epa.gov (J. Huang), mark.goltz@afit.edu (M.N. Goltz).

Recently, a more complete model that incorporates both scale-dependent dispersivity and molecular diffusion was presented by Haddad et al. (2015). In the Haddad et al. (2015) model the dispersion coefficient was represented as $(D = (ar + b)u(r) + D_m)$, where a and b are constants. The Haddad et al. (2015) model describes divergent flow of a conservative tracer from an injection well coupled with diffusive mass transfer of tracer into fractures.

In this study, a new analytical solution is developed that may be used to simulate contaminant transport in response to operation of a soil vapor extraction system. The model accounts for the following processes that affect VOC fate and transport in the vadose zone: (1) radial gas phase advection, (2) mechanical dispersion and effective molecular diffusion, (3) first-order degradation in gas, dissolved, and sorbed phases, and (4) rate-limited mass transfer between the gas phase and the dissolved/sorbed/NAPL phases. The model assumes the vadose zone is initially contaminated and the contaminated zone can be represented by a cylinder. The solution, which incorporates processes such as molecular diffusion and NAPL desaturation that were not considered in earlier models, can be employed to better understand how SVE performance is affected by various process parameter values.

2. Model equations

The conceptual model of SVE in a contaminated vadose zone is depicted in Fig. 1. In the vadose zone, voids are filled with air, water, and NAPL. Air containing volatilized contaminant is extracted through a fully screened well, while dissolved and NAPL phase contaminant volatilize into the gas phase. To mathematically describe the conceptual model, the following assumptions are made: 1) the vapor extraction well induces a steady, radially convergent gas flow field; 2) water and NAPL phases are immobile; 3) transport of volatilized contaminant in the vadose zone is governed by advection, dispersion and molecular diffusion; 4) contaminant mass transfer between phases can be described by first-order kinetics; 5) first-order decay of contaminant occurs in the dissolved, sorbed and volatilized phases; and, 6) saturation of NAPL is low, so that NAPL desaturation does not significantly change gas and water phase saturations, which are assumed constant.

Based on these assumptions, we modify Brusseau's (1991) one-dimensional formulation and Goltz and Oxley's (1991, 1994) radial flow model, to obtain the following equations describing the SVE process:

$$\theta s_g \frac{\partial C_g}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[(a_L q + r D_m) \frac{\partial C_g}{\partial r} + q C_g \right] + \alpha_{gw} (C_w - k_H C_g) + \alpha_{sg} (k_A C_s - k_H C_g) - \theta s_w \lambda_g C_g + R_E \quad (1)$$

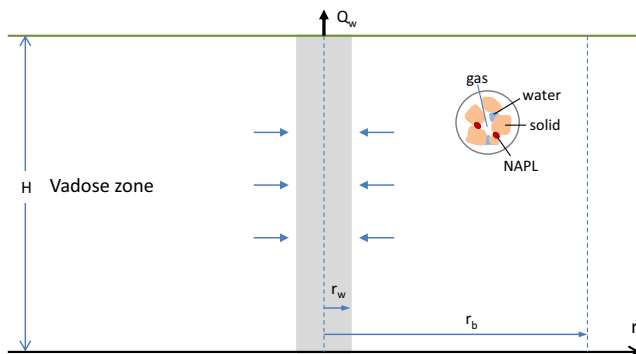


Fig. 1. Conceptual model for the soil vapor extraction.

$$\theta s_w \frac{\partial C_w}{\partial t} = \alpha_{gw} (k_H C_g - C_w) + \alpha_{ws} (k_A C_s - C_w) - \theta s_w \lambda_w C_w + R_D \quad (2)$$

$$\rho_b \frac{\partial C_s}{\partial t} = \alpha_{ws} (C_w - k_A C_s) + \alpha_{sg} (k_H C_g - k_A C_s) - \rho_b \lambda_s C_s \quad (3)$$

Eq. (1) describes the contaminant transport in the gas phase in the vadose zone; Eqs. (2) and (3) describe the interphase mass transfer. The subscripts g, w, s respectively refer to gas, water and solid phases; the subscripts gw, ws and sg respectively refer to interphase gas-water, water-solid and solid-gas; C is the contaminant concentration in gas, water or solid phase; θ is the porosity; s_g and s_w are respectively the gas and water saturation; ρ_b is the bulk density; $q = Q_w / (2\pi H)$, where Q_w is the well pumping rate and H is the thickness of the vadose zone; a_L is the longitudinal dispersivity in the gas phase; D_m is the effective molecular diffusion coefficient of contaminant in the gas phase; λ is the first-order decay constant of the contaminant, α is the non-equilibrium first-order mass transfer rate coefficient; k_H is the dimensionless Henry coefficient, expressed so $C_w = k_H C_g$; k_A is the adsorption partitioning constant, expressed so $C_w = k_A C_s$ at equilibrium; R_E is the volatilization rate of NAPL; R_D is the dissolution rate of NAPL; t is time; r is the radial coordinate.

The volatilization and dissolution of NAPL can be described by Eqs. (4a) and (4b) respectively, which assume first-order mass transfer processes in accordance with Raoult's Law:

$$R_E = s_n^\beta k_E (C_{equ} - C_g) \quad (4a)$$

$$R_D = s_n^\beta k_D (C_{sol} - C_w) \quad (4b)$$

where s_n is the saturation of NAPL; k_E is the volatilization rate coefficient of NAPL; C_{equ} is the equilibrium vapor concentration of NAPL in the gas phase; k_D is the dissolution rate coefficient of NAPL; C_{sol} is the solubility of NAPL in the water phase; and β is an empirical parameter characterizing the morphology of NAPL. To find an analytical solution for the SVE model, Eqs. (4a) and (4b) need to be linearized. Using the Taylor series expansion, neglecting the quadratic and higher order terms, Eqs. (4a) and (4b) may be approximated as:

$$R_E = k_E s_{nx}^\beta (C_{equ} - C_g) + k_E \beta s_{nx}^{\beta-1} (C_{equ} - C_{gx}) (s_n - s_{nx}) \quad (5a)$$

$$R_D = k_D s_{nx}^\beta (C_{sol} - C_w) + k_D \beta s_{nx}^{\beta-1} (C_{sol} - C_{wx}) (s_n - s_{nx}) \quad (5b)$$

where C_{gx} , C_{wx} and s_{nx} are, respectively, reference values of C_g , C_w and s_n . We select these reference values so that $\beta(C_{equ} - C_{gx}) = C_{equ}$, $\beta(C_{sol} - C_{wx}) = C_{sol}$ and $s_{nx} = s_{n0}$ (initial value of NAPL saturation) to guarantee that when the system is at equilibrium, the NAPL volatilization and dissolution rates go to zero. Using Eqs. (5a) and (5b), the NAPL desaturation equation then can be written as:

$$\begin{aligned} \theta \rho_n \frac{\partial s_n}{\partial t} &= -(R_E + R_D) \\ &= -k_E s_{n0}^{\beta-1} (C_{equ} s_n - s_{n0} C_g) - k_D s_{n0}^{\beta-1} (C_{sol} s_n - s_{n0} C_w) \end{aligned} \quad (6)$$

where ρ_n is the density of NAPL. The validity of this linearized NAPL desaturation model (6) to approximate the original non-linear Eqs. (4a) and (4b) is investigated in Section 4, Model Solution Verification. Note that neglecting the volume of NAPL in the pore space implies $s_g = 1 - s_w - s_n \approx 1 - s_w$.

Initial conditions are given by Eqs. (7a), (7b), (7c) and (7d), which assume all phases are initially at equilibrium.

$$C_g = C_{equ}, \quad t = 0 \quad (7a)$$

$$C_w = C_{sol}, \quad t = 0 \quad (7b)$$

$$C_s = \frac{1}{k_A} C_{sol}, \quad t = 0 \quad (7c)$$

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