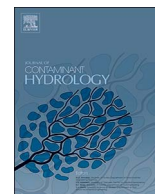




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Modelling mass transfer during venting/soil vapour extraction: Non-aqueous phase liquid/gas mass transfer coefficient estimation

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ABSTRACT

We investigate how the simulation of the venting/soil vapour extraction (SVE) process is affected by the mass transfer coefficient, using a model comprising five partial differential equations describing gas flow and mass conservation of phases and including an expression accounting for soil saturation conditions. In doing so, we test five previously reported equations for estimating the non-aqueous phase liquid (NAPL)/gas initial mass transfer coefficient and evaluate an expression that uses a reference NAPL saturation. Four venting/SVE experiments utilizing a sand column are performed with dry and non-saturated sand at low and high flow rates, and the obtained experimental results are subsequently simulated, revealing that hydrodynamic dispersion cannot be neglected in the estimation of the mass transfer coefficient, particularly in the case of low velocities. Among the tested models, only the analytical solution of a convection-dispersion equation and the equation proposed herein are suitable for correctly modelling the experimental results, with the developed model representing the best choice for correctly simulating the experimental results and the tailing part of the extracted gas concentration curve.

1. Introduction

Decontamination of the unsaturated zone of soil by evaporation of non-aqueous phase liquids (NAPLs) trapped at residual soil saturation is influenced by the soil vapour extraction (SVE)/venting process. Pollutant evaporation is promoted by the pressure gradient in the pores that induces the circulation of air in contact with NAPL. In the above zone, pollutants are present in several states: dissolved in residual saturation water, adsorbed on the organic matter and/or clay fraction of soil, and evaporated in the gas and/or water phase, with NAPL and aqueous phases considered to be non-mobile at residual saturation, in contrast to the gas phase experiencing a pressure gradient. The model used to simulate NAPL–gas phase transfer is based on mass conservation and convection diffusion (Eq. (1)):

$$\phi S_g \frac{\partial C_{g,\beta}}{\partial t} + \nabla [q_g C_{g,\beta}] - \nabla [\phi S_g \bar{D}_{g,\beta} \nabla C_{g,\beta}] = \phi S_g \lambda_{o-g,\beta} (C_{g,\beta}^{sat} - C_{g,\beta}) \quad (1)$$

where ϕ denotes porosity [–], S_g is the gas-phase saturation [–], q_g is the Darcy velocity in the gas phase [L T^{–1}], $\bar{D}_{g,\beta}$ is the hydrodynamic dispersion coefficient of compound β in the gas phase [L² T^{–1}], $\lambda_{o-g,\beta}$ is the coefficient of mass transfer between NAPL and the gas

phase for compound β [T^{–1}], and $C_{g,\beta}$ and $C_{g,\beta}^{sat}$ are the actual and saturation concentrations of compound β in the gas phase [M L^{–3}].

In this case, the physical parameters most important for studying transport/transfer are the NAPL–gas phase mass transfer coefficient (λ) and the longitudinal dispersion coefficient (α_L [L]). The α_L is included in the cinematic dispersion term which forms with diffusion term, the dispersion coefficient, whereas λ significantly influences the results obtained using the above model (Zhao, 2007). Indeed, the most difficult part of real-scale process simulation is finding a mathematical relationship for estimating this coefficient based on flow, porous media type, and pollutant characteristics/content. Duggal and Zytner (2009) simulated the experimental results obtained for two soils (Ottawa sand and Elora silt) at different extraction flow rates using a one-dimensional (1D) column (diameter = 6.8 cm, height = 20 cm) and a three-dimensional (3D) radial pilot (diameter = 40.5 cm, height = 51 cm, extraction well diameter = 3.2 cm). In the 1D column case for sand, the mass transfer coefficient was observed to be very high (944–250,000 h^{–1} for flow rates of 1.5–21.8 L·min^{–1}, respectively), being markedly lower for the pilot (4.5–43 h^{–1} at the same flow rates). The same behaviour was observed in our previous works (Boudouch et al., 2016), where we compared the results of model parameter identification for experiments performed using 3D pilots and 1D columns, considering the mass

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transfer to be constant in all subfields. This consideration was acceptable for a 1D approach, when pore velocity is homogeneous, whereas this velocity varied with distance from extraction wells at the radial pilot or field scale.

Previously, the mass transfer coefficient was estimated based on empirical models (van Genuchten and Alves, 1982; Wilkins et al., 1995; Yoon et al., 2002), with the most frequently used ones neglecting the longitudinal dispersion coefficient and not correctly estimating porous media saturation.

The coefficients of longitudinal dispersion and molecular diffusion determine the dispersion coefficient in the mass conservation equation (Eq. (1)), representing mechanical dispersion due to the heterogeneity of the fluid flow velocity in porous media. Dispersivity is an important pollutant transport property that is difficult to measure experimentally. However, it can be estimated from tracer breakthrough curves using analytical or numerical solutions of the mass conservation equation.

To evaluate the effect of saturation on the mass transfer coefficient, a typical extracted gas concentration curve given by the United States Environmental Protection Agency USEPA (1994) can be divided into three parts:

- the flushing phase, where the gas concentration is constant;
- the evaporation phase, corresponding to pollutant evaporation caused by contact between air and NAPL, where the concentration of extracted gas rapidly decreases;
- the diffusion phase, where the decrease of the mass transfer coefficient is attributed to the decreasing contact surface between phases.

This study aimed to propose a model for simulating the SVE/venting process, focusing on the effect of mass transfer coefficient evaluation on the simulation of experimental results, with four experimental SVE/venting tests performed. The developed model integrated the equation for calculating the mass transfer coefficient and was compared with five previously proposed mass transfer coefficient models to simulate experimental results. Finally, an additional expression taking saturation into account was proposed and tested.

2. Model

2.1. SVE/venting model

The SVE/venting model comprises five partial differential equations PDE, with the first being the continuity equation for gas flow simulation (Eq. (2)):

$$\frac{\partial(\phi S_g \rho_g)}{\partial t} + \nabla[\rho_g q_g] = Q_g^s + \sum_{\beta} E_{g,\beta} \quad (2)$$

where S_g is the saturation of the gas phase, ρ_g is the bulk density of the gas phase, q_g is the Darcy velocity, Q_g^s is the gas phase supply term [$M L^{-3} T^{-1}$], and $\sum_{\beta} E_{g,\beta}$ is the sum representing the transfer of all compounds β to the gas phase [$M L^{-3} T^{-1}$].

The remaining four equations simulate the mass conservation of gas, NAPL, aqueous, and immobile solid phases (Eq. (3)):

$$\frac{\partial}{\partial t}[\phi S_{\alpha} C_{\alpha,\beta}] + \nabla[q_{\alpha} C_{\alpha,\beta}] - \nabla[\phi S_{\alpha} \bar{D}_{\alpha,\beta} \nabla C_{\alpha,\beta}] = \sum_{\alpha} E_{\alpha,\beta} + Q_{\alpha}^s \quad (3)$$

where $C_{\alpha,\beta}$ is the concentration of compound β in phase α , S_{α} is the saturation of phase α , q_{α} is the Darcy velocity in phase α , and $\sum_{\alpha} E_{\alpha,\beta}$ is the sum representing the transfers of compound β to phase α [$M L^{-3} T^{-1}$]. $\bar{D}_{\alpha,\beta}$ [$L^2 T^{-1}$] is defined in Eq. (4) as:

$$\bar{D}_{\alpha,\beta} = \tau_{\alpha} D_{\alpha,\beta}^o \delta_{ij} + \left[\alpha_T |\vec{U}_{\alpha}| \delta_{ij} + (\alpha_L - \alpha_T) \frac{U_{ai} U_{aj}}{|\vec{U}_{\alpha}|} \right] \quad (4)$$

where $D_{\alpha,\beta}^o$ is the effective molecular diffusion coefficient of compound β in phase α [$L^2 T^{-1}$], δ_{ij} is the Kronecker symbol (equalling 1 if $i = j$, zero otherwise), α_L and α_T are the longitudinal and transversal dispersivities, respectively, U_{α} is the pore velocity of phase α [$L T^{-1}$], U_{ai} and U_{aj} are the pore velocities of phase α in directions i and j , respectively [$L T^{-1}$], and τ_{α} is the tortuosity factor calculated using the Milington model (Milington, 1959).

The volatilization or mass transfer between NAPL and gaseous phases was simulated using a first-order kinetic model (Eq. (5)):

$$E_{o-g,\beta} = \phi S_g \lambda_{o-g,\beta} (\bar{C}_{g,\beta}^{sat} - C_{g,\beta}) \quad (5)$$

where $E_{o-g,\beta}$ is the term describing NAPL-gas phase mass transfer for compound β [$M L^{-3} T^{-1}$], $\lambda_{o-g,\beta}$ is the corresponding coefficient of mass transfer [T^{-1}], and $C_{g,\beta}$ and $\bar{C}_{g,\beta}^{sat}$ are the equilibrium and saturation equilibrium concentrations of compound β in a mixture of gas phase [$M L^{-3}$].

The $(\bar{C}_{g,\beta}^{sat})$ was defined by Eq. (6):

$$\bar{C}_{g,\beta}^{sat} = \omega_{g,\beta} C_{g,\beta}^{sat} \quad (6)$$

where $C_{g,\beta}^{sat}$ is the concentration of compound β in the gas phase at equilibrium and saturation [$M L^{-3}$], and $\omega_{g,\beta}$ is the molar fraction of compound β in the gas phase [-].

Mass transfer between NAPL and aqueous phases was described by Eq. (7):

$$E_{o-w,\beta} = \phi S_w \lambda_{o-w,\beta} (S_{w,\beta}^{eff} - C_{w,\beta}) \quad (7)$$

where $S_{w,\beta}^{eff}$ is the effective solubility of compound β in the aqueous phase [$M L^{-3}$].

The NAPL/aqueous phase mass transfer coefficient can be calculated using the empirical correlation of the modified Sherwood number (Eq. (8)) (Miller et al., 1990):

$$Sh_{o-w,\beta}^m = \frac{\lambda_{o-w,\beta} d_{50}^2}{D_{w,\beta}^o} = 12 (\phi - \theta_o) Re_{w,\beta}^{0.75} \theta_o^{0.6} Sc_{w,\beta}^{0.5} \quad (8)$$

where $\lambda_{o-w,\beta}$ is the NAPL/aqueous phase mass transfer coefficient of compound β [T^{-1}], d_{50} is the mean diameter of soil grains [L], $D_{w,\beta}^o$ is the molecular diffusion coefficient of compound β in the aqueous phase [$L^2 T^{-1}$], θ_o is the volumetric content of the NAPL phase [$L^3 L^{-3}$], $Re_{w,\beta}$ is the Reynolds number of compound β in the aqueous phase, and $Sc_{w,\beta}$ is the Schmidt number of compound β in the aqueous phase.

To simulate mass transfer between aqueous and gas phases (stripping), the corresponding mass transfer coefficient was estimated from the empirical model of Chao et al. (1998) (Eq. (9)):

$$E_{w-g,\beta} = \phi S_w \lambda_{w-g,\beta} \left(C_{w,\beta} - \frac{C_{g,\beta}}{H_{\beta}} \right) = \phi S_w 10^{-2.49} D_{g,\beta}^{0.16} U_g^{0.84} d_{50}^{0.55} H_{\beta}^{-0.61} \left(C_{w,\beta} - \frac{C_{g,\beta}}{H_{\beta}} \right) \quad (9)$$

where $\lambda_{w-g,\beta}$ is the aqueous/gas-phase mass transfer coefficient of compound β [T^{-1}], $C_{w,\beta}$ is the concentration of compound β in the aqueous phase [$M L^{-3}$], U_g is the pore velocity of the gas phase [$L T^{-1}$], and H_{β} is the Henry constant of compound β [-].

To simulate mass transfer between aqueous and solid phases (sorption), the corresponding mass transfer coefficient was estimated using the empirical model of Brusseau and Rao (1989) (Eq. (10)):

$$E_{w-s,\beta} = \phi S_w \lambda_{w-s,\beta} \left(C_{w,\beta} - \frac{C_{s,\beta}}{K_{d,\beta}} \right) = \phi S_w \text{Exp} (0.301 - 0.668 \log(K_{d,\beta})) \left(C_{w,\beta} - \frac{C_{s,\beta}}{K_{d,\beta}} \right) \quad (10)$$

where $C_{s,\beta}$ is the concentration of compound β in the solid phase [$M L^{-3}$], and $K_{d,\beta}$ is the sorption coefficient of compound β in soil [$L^3 M^{-1}$]. In this work the sorption on solid phase is produced only by the

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