Journal of Contaminant Hydrology 147 (2013) 82–95

Contents lists available at SciVerse ScienceDirect

Journal of Contaminant Hydrology

journal homepage: www.elsevier.com/locate/jconhyd

Three-dimensional numerical model for soil vapor extraction

Van Thinh Nguyen [a], Lian Zhao [b], Richard G. Zytner [c,*]

[a] Department of Civil and Environmental Engineering, Seoul National University, Republic of Korea
[b] Integrated Environments (2006) Ltd., 2509 Dieppe Ave. SW, Calgary, AB, Canada T3E 7J9
[c] School of Engineering, University of Guelph, Guelph, ON, Canada N1G 2W1

ARTICLE INFO

Article history:
Received 26 April 2012
Received in revised form 14 February 2013
Accepted 15 February 2013
Available online 24 February 2013

Keywords:
Soil vapor extraction
3D numerical model
Multiphase flow
Multi-component transport
Rate-limited mass transfer

ABSTRACT

Mass transfer limitations impact the effectiveness of soil vapor extraction (SVE) and cause tailing. In order to identify the governing mass transfer processes, a three-dimensional SVE numerical model was developed. The developed model was based on Comsol Multiphysics® a finite element method that incorporates multi-phase flow, multi-component transport and non-equilibrium transient mass transfer. Model calibration was done against experimental data from previously completed lab-scale reactor experiments.

The developed model, 3D-SVE, nicely simulates laboratory findings and allows for changes in the important governing mass transfer relationships. The modeling results showed that a single averaged mass transfer value is a poor representation of the entire SVE operation, and that a transient mass transfer coefficient is required to fully represent SVE tailing. Calibration of the lab scale model showed that the most important mass transfer occurs between the NAPL and vapor phase.

1. Introduction

Numerical modeling has become an important tool in the development of SVE technology by providing a better understanding of the SVE processes, and enhancement of SVE applications (Barnes, 2003; Barnes and White, 2006; Bradner and Murdoch, 2005; Harper et al., 2003) A proper numerical model can also assist in the design of an SVE system (Thomson et al., 1997), and help evaluate when SVE should be stopped (Carroll et al., 2012; Zhao and Zytner, 2008). Unfortunately, very few models incorporate transient mass transfer processes in a three-dimensional setting, which adversely affects performance. As such, most designs are based on either simple "rule-of-thumb" estimations, analytical approximations or limited simulations, which lead to model deficiencies when simulating real world SVE situations (Brusseau et al., 2010; Rahbeh and Mohtar, 2007; Rathfelder et al., 2000).

Some studies have focused on specific non-equilibrium mass transfer processes in one-dimensional (1D) column or two-dimensional (2D) horizontal experiments and numerical investigations (Abriola et al., 1997; Carroll et al., 2012; Høier et al., 2009; Rathfelder et al., 2000). The problem is, 1D/2D models cannot simulate the complex fluid flows and transport processes in subsurface soils with high heterogeneity. However, three-dimensional (3D) models may produce a markedly improved remediation design due to the following reasons. First, modeling in 3D may use all the information available from actual spatially variable characteristics of the subsurface site, by using detailed soil mapping processes and ultimately conducting experiments with contaminated soil. Hence predictions may be improved. Secondly, due to the inclusion of SVE configurations and operation conditions, modified multiphase, multi-component and non-equilibrium 3D models would be possible, giving more realistic predictions than local equilibrium models or one- or two-dimensional models. Development of these three-dimensional models with variable inputs can then be the starting point of extending the results to field settings, despite the requirement for significant input data and large computational requirements.

The ability of a 3D SVE model to match real field performance data is the most difficult, specifically within the tailing region

* Corresponding author. Tel.: +1 519 824 4120; fax: +1 519 836 0227.
E-mail address: rzytner@uoguelph.ca (R.G. Zytner).

0169-7722/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.jconhyd.2013.02.008

(Barnes and White, 2006). Rate-limited mass transfer is an important factor that impacts tailing (Chai and Miura, 2004; Gidda et al., 2011), and the efficiency and speed of remediation (Carroll et al., 2012; Zhao and Zytner, 2008). Accordingly, the inclusion of rate-limited mass transfer coefficients within the 3D model is paramount to accurately simulating real field scenarios. There have been some multiphase flow and multi-component transport mathematical models dealing with SVE processes incorporating interface mass transfer documented in the literature, such as Sleep and Sykes (1989, 1993), Lingineni and Dhir (1997), Abriola et al. (1997, 1999), Thomson et al. (1997) and Rathfelder et al. (2000).

The USACE (2002) reported several 3D models for soil vapor extraction, but these models have been used only to simulate air flow and design the SVE system by screening the candidacy of a site and arranging the layout of wells. MODFLOW is a three-dimensional finite-difference groundwater model; connected to GMS (Groundwater Modeling System). It is often used in SVE simulation, assuming a single gas phase flow, whereas water and NAPL phases are immobile. AIR3D was developed to estimate the unsaturated zone permeability from field data obtained from horizontal well SVE tests. AIR3D is an adaptation of the groundwater flow code MODFLOW to simulate 3D air flows in a heterogeneous, anisotropic unsaturated zone where air flow is induced through dry wells or trenches, as in vapor extraction remediation. GAS2D and GAS3D are numerical two- and three-dimensional models developed to simulate gas flow conditions under vadose zone conditions. The GAS3D model was verified and validated by comparing the results of the finite-difference solution to actual field measurements and the results of an analytical solution under homogeneous and isotropic conditions without transport of contaminants.

At present time, two commercially available 3D vapor flow and transport models are VENT3D (Benson, 2011) and SVE-3D (Scientific Software Group, 2011). A comparison on the ability of the developed model with other 3D numerical models is shown in Table 1.

The 3D model developed in this study simulates multiphase flow in a multi-component transport situation and incorporates non-equilibrium transient mass transfer. The model provides the foundation for more complex simulations like multi-well spacing. Calibration was done against the sets of 3D experimental data (Duggal and Zytner, 2009), using mass transfer coefficients as fitting parameters. A comparison of the numerical results with the experimental data shows very good agreement. Multi-variable sensitivity analysis was also implemented to determine which parameter had the most impact on the simulation, to give a better understanding of the dominant mechanisms contributing to the long tailing effects in SVE operation.

2. Methodology

2.1. Setting up the 3D-SVE model

Using a suitable conceptual model to represent SVE operation is crucial when conducting modeling studies. A typical contaminated site is considered to be a heterogeneous domain. The installation of injection or passive wells improves the flow of fresh air, while sealing the ground surface of a contaminated zone overcomes the by-pass of air flow around the venting well. Three-dimensional modeling allows the simulation of a complete SVE system under these practical operational conditions and geological settings.

SVE treatment utilizes the volatile properties of contaminants, whereby mass transfer occurs between the adsorbed, dissolved, and free phases in the soil and vapor phases. The contaminants which are converted into vapor phase will be removed through the venting well and treated aboveground. The numerical model integrates the processes identified in three-phase flow and multi-component compositional transport by incorporating non-equilibrium interphase mass transfer.

Initially, the spilled NAPL in the soil starts in the pure NAPL phase (referred to as residual saturation), from which

Table 1
Comprehensive comparison of 3D models.

Models	3D-SVE	SVE-3D	VENT3D	Other models
Developer	Authors of this paper	Scientific Software Inc. (2011)	Benson (2011)	Sleep and Sykes (1989), Abriola et al. (1997) Rathfelder et al. (2000) Thomson et al. (1997)
Numerical scheme	Finite element FEMLAB	Finite element	Finite difference	Finite difference or finite element
User adaptation	√	X	X	X
Heterogeneous permeability	√	√	√	Limited
Multicomponent	√	√	√	√
Phases	4 phases, single gas active phase flow	4 phases, three phase flow	Gas phase only	Aqueous and gas phase flow
Mass transfer	Nonequilibrium Transient mass transfer coefficients	Nonequilibrium, constant mass transfer coefficients	Equilibrium	Nonequilibrium Constant mass transfer coefficients
Special features	Predict closure time and degree of final cleanup	Estimate number of SVE wells, wells' spacing, and cleanup time under complex conditions	Third-order vapor transport algorithm	Model-dependent
Calibration	√	√	√	√
Adjustable parameters	Mass transfer empirical parameters	first order biodegradation simulated	Initial concentration	Intermodel, analytical solution