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ScienceDirect
Journal of Hazardous Materials 143 (2007) 156–170
Journal of Hazardous Materials
www.elsevier.com/locate/jhazmat

Application of multiphase transport models to field remediation by air sparging and soil vapor extraction

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Received 13 September 2004; received in revised form 26 June 2006; accepted 4 September 2006
Available online 9 November 2006

Abstract

The design and operation of air sparging and soil vapor extraction (AS/SVE) remediation systems remains in large an art due to the absence of reliable physically based models that can utilize the limited available field data. In this paper, a numerical model developed for the design and operation of air sparging and soil vapor extractions systems was used to simulate two field case studies. The first-order mass transfer kinetics were incorporated into the model to account for contaminant mass transfer between the water and air (stripping), NAPL and water (dissolution), NAPL and air (volatilization), and water and soil (sorption/desorption), the model also accounted for soil heterogeneity. Benzene, toluene, ethyl benzene and xylenes (BTEX) were the contaminants of concern in both case studies. In the second case study, the model was used to evaluate the effect of pulsed sparging on the removal rate of BTEX compounds. The pulsed sparging operation was approximated assuming uniform contaminant redistribution at the beginning of the shut-off period. The close comparison between the observed and simulated contaminant concentration in the aqueous phase showed that the approximation of the pulsed sparging operation yielded reasonable prediction of the removal process. Field heterogeneity was simulated using Monte Carlo analysis. The model predicted about 80–85% of the contaminant mass was removed by air–water mass transfer, which was similar to the average removal obtained by Monte Carlo analysis. The analysis of the removal/rebound cycles demonstrated that removal rate was controlled by the organic–aqueous distribution coefficient K_{oc}. Due to the lack of site-specific data, the aerobic first-order biodegradation coefficients (k_{bio}) were obtained from a literature survey, therefore, uncertainty analysis of the k_{bio} was conducted to evaluate the contribution of the aerobic biodegradation to total contaminant removal. Results of both case studies showed that biodegradation played a major role in the remediation of the contaminated sites.

Keywords: Air sparging; Biodegradation; Pulsed sparging; Mass transfer; Field remediation

1. Introduction

The introduction of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) of 1980 [1] created the need for the evaluation and treatment of contaminant plumes caused by accidental spills of industrial waste. The need for multiphase flow and transport models became even more pressing after the development of remediation techniques that require the injection of remedial fluids such as co-solvents, or techniques that involve remediation by advective air flux such air sparging (AS) and/or soil vapor extraction (SVE).

Multiphase flow and transport modeling is a well-known practice in the petroleum engineering, however, the different motivation of the petroleum and environmental engineering promoted the development of models that are generally aimed at the characterization of the contaminant plume [2–5], and the simulation and design of remediation systems [6–10]. Abriola and Pinder [11] demonstrated their model [2] by modelling the one-dimensional hypothetical infiltration of a hydrocarbon mixture into a soil column. Sleep and Sykes [12] considered a hypothetical distribution of organic contaminant in the subsurface. Baehr and Corpcioglu [13] used a one-dimensional approximation to evaluate, hypothetically, the transport of organic contaminant from the unsaturated zone into ground water. Unger et al. [8] and Rathfelder et al. [10] applied their models to hypothetical AS/SVE problems. All of these models and research articles provided an excellent discussion and insight for the numerical

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doi:10.1016/j.jhazmat.2006.09.098

solution of multiphase systems, however, without application to field case studies, Radideau et al. [14] and Benner et al. [15] applied semi-empirical models to field case studies. Semi-empirical models, however, require an on-site pre-calibration of an existing air sparging system before it can be used. In this case, the model cannot be used for the design and feasibility studies, and cannot be used for short-term operations, which may defeat the purpose of the model in the first place.

Our objective is to demonstrate the use of a practical and efficient model in the evaluation of two AS/SVE field case studies. The main advantage of the model is its flexibility to take advantage of the limited amount of data that are usually available, while retaining the ability to simulate the processes that contribute to the overall contaminant removal. The analysis for the first case study focuses on the effect of natural attenuation on the contaminant removal processes. The second case study addresses the issues of heterogeneity and pulse sparging, a technique that is usually used to enhance the performance of AS systems.

2. Methodology

2.1. Model description

The unsaturated air flow and contaminant transport model uses first-order kinetics to represent the mass transfer among the aqueous, gaseous, solid, and NAPL phases. The model accounts for heterogeneous domains and considers distinguished single-phase and multi-phase domains. This capability is especially important in the case of remediation techniques that involve an advective air flux such as air sparging and soil vapor extraction. In such systems, two domains may be considered, the advective domain, i.e. the air, and the non-advective domain, which may be either the domain outside the advective air domain but in the vicinity of the air-plume, or any space or pocket inside the advective air domain that is not in direct contact with the advective air domain. The model consists of two main modules; the first module, the steady state unsaturated flow that solves for air flow, uses air permeability as an input and determines the capillary pressure head distribution. The flow module can consider air injection (air sparging) by imposing positive pressure as a fixed boundary condition at the sparging well. Likewise, negative pressure can be imposed to represent extraction (SVE). The second module, multiphase contaminant transport, incorporates first-order mass transfer kinetics to model the contaminant mass transfer among all phases involved: namely, the aqueous, gaseous and, solid phases. The flow and transport simulations are decoupled such that the steady state air flow is determined first, and then the pressure heads are interpolated to the transport model.

2.1.1. The steady unsaturated flow module

AS and/or SVE are usually applied to remove trace and residual contaminant concentrations rather than removing the NAPL free phase. In practice neither free flowing light non-aqueous (LNAPL) nor dense non-aqueous phase (DNAPL) have been detected at sites where an advective air flux technology has been used as a remediation technique [16,17]. Furthermore, it has been found that the effect of ground water flow on the size and shape of ROI is negligible [18], and that the time required for an AS to reach steady state is negligible relative to the average operational time [16,18]. For SVE applications, Massmann [19] treated the air flow as saturated, i.e. single phase flow, by ignoring the effect of the soil moisture condition in the vadose zone. Sawyer and Kamakoti [20], realizing the analogy between flow equations, went one step further and used MODFLOW as a design tool for SVE systems. In this paper, we used the unsaturated steady state flow model SPARG, developed by Mohtar et al. [21], to supplement the transient multiphase model. This involved the assumption of instantaneous attainment of the steady state conditions, which may incur some error at the beginning of simulation. However, it allowed independent simulation for the transport and flow components, thus saving substantial effort and computational time.

2.1.2. Multiphase transport module

The multiphase contaminant transport model uses first-order mass transfer kinetics, $\mathrm{d}C/\mathrm{d}t = k_\mathrm{f}(C - C_\mathrm{aq})$, to represent mass transfer among the aqueous, gaseous, solid and NAPL phases. The theoretical basis of the multiphase transport model is founded on the concept that a polar liquid wets a polar surface in preference to non-polar liquid, therefore, water preferentially wets soil particles, thus preventing a direct contact between the soil particles and intruding non-aqueous phase or advecting gaseous phase. This has been demonstrated by Wilson et al. [22] using etched glass micro models to visualize the distribution of non-aqueous phase liquid (NAPL), water and air phases. They concluded that the glass was always surrounded by a thin film of water as the air and water were in contact with each other, but not with the glass which represented the soil particle in an actual porous medium. Therefore, the contaminant mass transfer can take place across the aqueous–solid (sorption/desorption), aqueous–gaseous (stripping), aqueous–NAPL (dissolution), and gaseous–NAPL (volatilization) interfaces. In the context of remediation by AS/SVE, the mobile phases may be restricted to the aqueous and gaseous phases only. However, the model incorporates a seepage process in terms of a first-order sink term in order to relax the stationary aqueous phase assumption, and to compensate for the contaminant movement due to the gentle slope in the water table.

2.1.3. Governing equations

The governing equations are based on the concept of conservation of mass and volume averaging, or the representative equivalent volume (REV) [23], which has been extensively used in multiphase contaminant transport models including those involving an advective gaseous phase.

Accordingly, the governing equation for the contaminant transport in the aqueous phase is written as (e.g., Fetter [24]):

$$\frac{\partial C_{\mathrm{aq}}^{\alpha}}{\partial t} = \nabla J_{\mathrm{aq}_i}^{\alpha} - R_{\mathrm{stripping}}^{\alpha} - R_{\mathrm{soprtion/desorption}}^{\alpha} + R_{\mathrm{dissolution}}^{\alpha} - \kappa C_{\mathrm{aq}}^{\alpha} - \beta C_{\mathrm{aq}}^{\alpha}, \quad i = 1, 2 \qquad (1)$$