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A three-dimensional numerical model for linking community-wide vapour risks

Nizar Mustafa [a], Kevin G. Mumford [b,*], Jason I. Gerhard [a], Denis M. O'Carroll [a]

[a] Department of Civil and Environmental Engineering, University of Western Ontario, London, Ontario N6A 5B9, Canada
[b] Department of Civil Engineering, Queen's University, Kingston, Ontario K7L 3N6, Canada

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ABSTRACT

A three-dimensional (3D) numerical model that couples contaminant transport in the saturated zone to vapour transport in the vadose zone and vapour intrusion into buildings was developed. Coupling these processes allows the simulation of vapour intrusion, arising from volatilization at the water table, associated with temporally and spatially variable groundwater plumes. In particular, the model was designed to permit, for the first time, 3D simulations of risk at receptors located in the wider community (i.e., kilometre scale) surrounding a contaminated site. The model can account for heterogeneous distributions of permeability, fraction organic carbon, sorption and biodegradation in the vadose and saturated zones. The model formulation, based upon integration of a number of widely accepted models, is presented along with verification and benchmarking tests. In addition, a number of exploratory simulations of benzene and naphthalene transport in a 1000 m long domain (aquifer cross-section: 500 m × 14 m) are presented, which employed conservative assumptions consistent with the development of regulatory guidance. Under these conservative conditions, these simulations demonstrated, for example, that whether houses in the community were predicted to be impacted by groundwater and indoor air concentrations exceeding regulatory standards strongly depended on their distance downgradient from the source and lateral distance from the plume centreline. In addition, this study reveals that the degree of reduction in source concentration (i.e., remediation) required to achieve compliance with standards is less if the risk receptor is in the wider community than at the site boundary. However, these example scenarios suggest that, even considering community receptors, sources with initially high concentrations still required substantial remediation (i.e., >99% reductions in source concentration). Overall, this work provides insights and a new tool for considering the relationships between contaminated site source zones and community-wide risk assessment that allows for development of policies and technical approaches for contaminated site management. It is anticipated that this coupled model not only will allow significant convenience, for example in running suites of Monte Carlo simulations for complex scenarios, but will also allow the investigation of vapour intrusion under conditions where soil gas concentrations may change over the same timescale as an evolving plume.

1. Introduction

Contaminated groundwater associated with improper handling or disposal of hazardous industrial liquids such as nonaqueous phase liquids (NAPLs) is common, with adverse effects on the environment and human health. Risk assessment is a critical tool for quantifying the potential impacts and has become widely used to support regulatory frameworks and site-specific decisions (e.g., Ma, 2002; Maxwell and Kastenberg, 1999). For sites contaminated with volatile organic compounds (VOCs), vapour intrusion into buildings has emerged as a critical component of risk assessments, and

* Corresponding author. Tel.: +1 613 533 6325; fax: +1 613 533 2128.
E-mail address: kevin.mumford@civil.queensu.ca (K.G. Mumford).

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thereby a controlling factor in determining mitigation and remediation activities (Abreu and Johnson, 2005, 2006; Bozkurt et al., 2009; DeVault et al., 2002; Fischer et al., 1996; Hers et al., 2001; Johnson and Ettinger, 1991; Lahvis et al., 1999; Ostendorf and Kampbell, 1991; Roggemans et al., 2002; Wang et al., 2012; Yao et al., 2013; Yu et al., 2009).

In many jurisdictions soil and groundwater standards for VOCs have been established using risk-based criteria applied at the boundaries of the contaminated site; for example, in Ontario, Canada this distance is assumed to be 43 m. However, often the critical contaminant pathways and risk receptors are in the adjacent community at distances greater than these assumed site boundary distances. Confining risk assessments to the site boundaries may be overly conservative in some cases, requiring remediation to a degree that is technically impractical, and thereby impeding brownfield redevelopment. Risk-based approaches evaluated at the community level may reveal significantly different compliance criteria than the standard approach at the property level, supporting achievable site closure while still remaining protective of human health (e.g., Malina et al., 2006; Weiss et al., 2006; Wycisk et al., 2003). Conducting community-based (or 'area-wide') risk assessment studies, therefore, requires the ability to predict a number of contaminant pathways at the community scale, including those related to groundwater and vapour intrusion.

Models to simulate vapour intrusion have been developed and widely used (e.g., Abreu and Johnson, 2005; Bozkurt et al., 2009; DeVaull et al., 2002; Johnson and Ettinger, 1991). Some of these models are based on analytical solutions and necessarily employ simplified assumptions about the scenario (e.g., homogeneous subsurface, one-dimensional geometry), which can limit their applicability to more complex site conditions. Numerical models (Abreu and Johnson, 2005, 2006; Abreu et al., 2009; Bozkurt et al., 2009) are able to overcome some of these restrictions, employing three-dimensional domains to consider the vapour pathway from the water table to the bottom of the basement slab and then to indoor air. These models are capable of simulating a wide range of conditions (USEPA, 2012); however, studies that have used these models have typically focused on smaller domains (e.g., up to 100 m × 100 m) with uniform, constant-concentration sources located either directly below or laterally offset from the building foundation. These conditions may not be applicable to community-scale scenarios where groundwater plumes extend over larger distances and concentrations will be temporally variable near each house. For example, the time required for soil gas concentration profiles to reach steady-state may be on the scale of changes in groundwater concentrations for plumes not at steady state, particularly for fine-grained soils with high sorption (USEPA, 2012) or where biodegradation in the vadose zone is significant. Under these conditions, coupling evolving groundwater concentrations to soil gas concentrations and vapour intrusion would be advantageous.

Yu et al. (2009) employed a multiphase, multi-component model to examine the fate of trichloroethylene (TCE) vapours from a NAPL source zone in a heterogeneous aquifer. Their sensitivity studies explored the influence of capillary fringe thickness, slab fracture aperture, infiltration rate, and indoor air pressure drop within the house. The numerical model included significant complexity in processes (e.g., NAPL migration, heterogeneity in the subsurface, contaminant transport across a capillary fringe, and pressure fluctuations in the indoor air). As a result, their study employed some simplifications in order to achieve manageable simulation times, such as (i) a two-dimensional cross-section domain, (ii) equilibrium mass transfer between phases, (iii) no sorption in the vapour phase, and (iv) no degradation in the water and the vapour phases. In addition, the domain size in that study was limited to the immediate vicinity of the source zone such that the receptor was 50 m downgradient and the aquifer was only 8 m deep. Wang et al. (2012) performed additional simulations using the model of Yu et al. (2009), which were extended to three dimensions and investigated multiple houses in domains 160 m long × 50 m wide × up to 15 m deep.

The goal of this study was to investigate the prediction of risk from VOC-contaminated sites on groundwater and vapour receptors in the surrounding community and to demonstrate a coupled modelling approach to asses these receptors within the same simulation. The specific objectives of the study were to (i) consider the difference in the degree of source zone remediation required when risk assessment was conducted at the site boundary versus at receptors in the community, and (ii) evaluate the sensitivity of this difference to two factors: the physicochemical properties of the contaminant (comparing benzene and naphthalene), and whether groundwater or indoor air was considered the risk driver. In this study, risk was assessed by comparing groundwater and indoor air concentrations against a regulatory standard. In order to pursue these objectives, a new numerical model, GW-VAP3D, was developed. This model couples three existing models to simulate three-dimensional contaminant transport in both groundwater and vapour phases, including (i) sorption and biodegradation in both phases, (ii) vapour intrusion into buildings, and (iii) spatial heterogeneity of subsurface parameters (e.g., hydraulic conductivity, fraction organic carbon). One novel feature of this model is that it is designed to be computationally inexpensive even for community-scale domains (i.e., on the scale of 100's to 1000's of metres). Seven example simulations were conducted to demonstrate this new model using conditions similar to those used to develop regulatory standards in Ontario, Canada which are designed to be protective of human health and the environment (MOE, 2011). As such, the simulation conditions used here are necessarily very conservative and are not intended to be representative of typical contaminated sites. However, it is expected that the approach will be of interest to other jurisdictions interested in risk-based approaches applied at a community level (e.g., Malina et al., 2006; Weiss et al., 2006; Wycisk et al., 2003).

2. Model development

2.1. Conceptual framework

An example contaminated site is shown in Fig. 1, where a NAPL below the water table presents a long-term contamination source. Dissolution of the NAPL generates an aqueous plume of VOCs subject to volatilization to the soil gas in the vadose zone, and both the aqueous and gaseous VOC plumes are subject to advection, dispersion, sorption and biodegradation. In the vadose zone, pressure differences between the interior of buildings and the subsurface induce flow of