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Simulating an exclusion zone for vapour intrusion of TCE from groundwater into indoor air

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ABSTRACT

This paper is an extension of the work by Yu et al. (2009) to examine exposure pathways of volatile organic compounds (VOCs) originating from a NAPL source zone located below the water table, and their potential impact on multiple residential dwellings down-gradient of the source zone. The three-dimensional problem geometry is based on the Rivett (1995) field experiment in the Borden aquifer, and contains houses located both above and adjacent to the groundwater plume in order to define an exclusion zone. Simulation results using the numerical model *CompFlow Bio* indicate that houses which are laterally offset from the groundwater plume are less affected by vapour intrusion than those located directly above the plume due to limited transverse horizontal flux of TCE within the groundwater plume, in agreement with the ASTM (2008) guidance. Uncertainty in the simulated indoor air concentration is sensitive to heterogeneity in the permeability structure of a stratigraphically continuous aquifer, with uncertainty defined as the probability of simulated indoor air concentrations exceeding the NYSDOH (2005) regulatory limit. Within this uncertainty framework, this work shows that the Johnson and Ettinger (1991), ASTM (2008) and *CompFlow Bio* models all delineate an identical exclusion zone at a 99.9% confidence interval of indoor air concentrations based on the probability of exceedence.

1. Introduction

Numerous sites with monitored shallow groundwater plumes originating from volatile organic contaminant source zones also exhibit deleterious impacts on the vadose zone immediately above the plume (Rivett, 1995; Smedes et al., 1993). This issue is problematic given the potential for vapour intrusion of the volatile organic contaminants to adversely impact the indoor air quality of houses with foundation slabs located within the area of impacted vadose zone. To address this issue, two layers of regulatory guidance have been developed. In the first level, the concepts of "exclusion criteria" and an "exclusion distance" are defined relative to the geometry of the groundwater plume and other characteristics of the site, provide the rationale to exclude the need to conduct further pathway assessment and monitoring, and characterize the house as being unaffected by the subsurface contamination (Luo et al., 2010). For the scenario where the vapour source is a non-biodegradable volatile organic groundwater plume, ASTM (2008) (Section 8.5.3) itemizes the critical distance demarking the exclusion zone as being 100 ft (approximately 30 m) from the perimeter of the plume. This critical distance is adjusted whether, for instance, the source of the vapours is a dissolved and biodegradable hydrocarbon plume, or even a NAPL source zone. In the second level, science-based regulatory criteria are used to evaluate the fate and transport of volatile organic contaminants from the subsurface into the indoor air of residential dwellings. In particular, the Johnson and Ettinger (1991) heuristic model (the J&E model) has become the de-factor standard. While designed to be conservative (Fitzpatrick and Fitzgerald, 2002; Hers et al., 2003; Johnston and Gibson, 2011; Mills et al., 2007; Provoost et al., 2010; Schreuder, 2006; USAF, 2006; Yu et al., 2009), the J&E model was also found to be the most accurate and least conservative

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in comparison to six other methodologies used in Europe (Provoost et al., 2009). Despite numerous simplifying assumptions used to develop the closed-form analytical solution constituting the J&E model, limited site characterization budgets have motivated its wide-spread application as a preliminary screening tool to virtually all sites in the United States and Canada. Given a regulatory limit defining the maximum permissible indoor air concentration (NYSDOH, 2005; OEHHA-CEPA, 2007, the J&E model can then be as an alternative to ASTM (2008) to identify those residential dwellings that are unlikely to be adversely affected by subsurface contamination and hence are within the exclusion zone.

While the use of the J&E model to define an exclusion zone is a straightforward extension of its current scope of application, alternative models could also be used to include additional science-based mechanisms controlling the fate and transport of contaminants from the subsurface into the indoor air further refining the geometry of the exclusion zone. Yu et al. (2009) used the numerical model *CompFlow Bio* to simulate the fate and transport of TCE from groundwater to indoor air. This work adopts Fig. 1b of Yu et al. (2009) as the problem geometry under the assumption that the pathway for the contamination from the source zone into the indoor air is advective and diffusive transport in the groundwater (see Gillham et al., 1984) from the NAPL source zone to beneath the foundation slab of the residential dwelling, upward diffusive transport across the capillary fringe into the vadose zone, and advective and diffusive transport in the gas phase within the vadose zone through a crack in the foundation slab and into the residential dwelling. This problem geometry was motivated by a field experiment conducted by Rivett (1995) in the Borden aquifer, who observed that weak vertical transverse transport resulting from hydrodynamic dispersion below the water table allows the groundwater plume to transport contaminants without mass transport across the capillary fringe. McCarthy and Johnson (1993) conducted a laboratory experiment and observed that vertical mass transport of contaminants across the capillary fringe was controlled by aqueous phase diffusion.

Within the last two decades, numerical modeling tools have evolved significantly to help interpret and parameterize the physical processes controlling the fate and transport of contaminants from groundwater into the vadose zone. Early models such as those by Mendoza and Frind (1990a, 1990b), Culver et al. (1991), Celia and Binning (1992) and Thomson et al. (1997) focused on mathematical formulation and model development issues to adequately represent this transport mechanism. Later models evolved to focus on soil vapour intrusion pathways, including: the effect of atmospheric pressure (Massmann and Farrier, 1992), and the effect of wind speed and direction (Riley et al., 1999). Parker (2002) and DeVaull et al. (2002) emphasized the significance of biodegradation, while Abreu and Johnson (2005, 2006) then included biodegradation processes into a three-dimensional numerical model to investigate the impact of building construction, degradation rate, and the NAPL source zone architecture on indoor air concentrations. Robinson and Turczynowicz (2005) and Bozkurt et al. (2009) also use fully three-dimensional problem geometries, with the latter examining the impact of multiple stratigraphic units on the fate and transport of contaminants through the vadose into the indoor air. Abreu and Johnson (2005) and Lowell and Eklund (2004) focus on the issue of lateral source zone separation which has direct relevance to the issue of defining an exclusion zone. Yu et al. (2009) used a two-dimensional numerical mesh to simulate the fate and transport of contaminants from groundwater to indoor air. They hypothesized that the resulting indoor air concentrations would be conservative given that the groundwater plume was forced to be transported beneath the foundation slab of the house, and the lack of transverse horizontal transport to the groundwater plume could not reduce groundwater concentrations within the plume. Given this limitation in the numerical mesh, they were unable to conclude whether the J&E model generated conservative indoor air concentrations relative to their simulation results. At present, we are unaware of any previous efforts to simulate the fate and transport of contaminants from groundwater, through the vadose zone and into the indoor air for multiple residential dwellings. The last criterion is essential when attempting to use a numerical model to help delineate an exclusion zone, with houses directly above and laterally offset from the surface projection of the groundwater plume.

The objective of this work is to use the multi-phase compositional numerical model *CompFlow Bio* to examine the fate and transport of volatile organic contaminants originating from a NAPL source zone located below the water table, and their potential impact on multiple residential dwellings located down-gradient of the source zone. The problem geometry is based directly on Fig. 1b of Yu et al. (2009) and hence is based on the Rivett (1995) field experiment in the Borden aquifer. In this work, the problem geometry is extended to be fully three-dimensional. This enhancement was motivated by the need to accommodate the multiple houses, with some laterally offset from the direction of groundwater plume advection, in an attempt to delineate an exclusion zone. This enhancement also permits the evaluation of the transverse horizontal flux of contaminant (to the direction of the groundwater plume advection) on reducing contaminant concentrations within the plume and ultimately within the indoor air. Following the discussion by Yu et al. (2009) detailing the methodology for comparing the *CompFlow Bio* and J&E models, we can then further refine statements in Yu et al. (2009) regarding the conservative nature of the J&E model.

2. Conceptual and numerical model

The conceptual and numerical model used in this study is largely an extension of that initially presented in Yu et al. (2009). As such, development of the conceptual and numerical model consists of two stages. First, this work outlines the formulation of the three-phase multi-component compositional numerical model *CompFlow Bio* to solve the relevant governing equations and constitutive relationships to simulate the fate and transport of TCE emanating from a non-aqueous phase source zone located in a variably saturated aquifer. In this case, the pathway includes dissolution of TCE into the ambient groundwater, mass transfer across the capillary fringe, and subsequent advective-dispersive transport in the mobile soil gas and groundwater towards the foundation slab of multiple structures located below grade. Second, this work develops a conceptual model of the variably saturated aquifer,