

# Chapter 1

## Developing Vapor Intrusion Models

### 1.1 Introduction

No models are true representations of reality, but some of them may be useful. Ever since Newton first wrote his laws of motion, mankind has tried to describe reality with an ever increasing number of mathematical statements. With the advent of computation and advancements in numerical methods our capabilities to mathematically describe physical systems has dramatically increased. Even so, real-world systems are too complex to be fully modeled, but mathematical representations may be used to approximate and reveal useful insights of how they function.

This is especially true for vapor intrusion (VI) models. Often it is impossible or difficult to conduct controlled studies of VI sites making models an important tool for understanding these sites and the VI phenomena. The previous chapter is proof of this as it is readily apparent that a multitude of VI models of varying complexity have been developed over the years, and has become an important part of the scientific VI community. From the simple Johnson & Ettinger one-dimensional model to full three-dimensional finite element models (FEM) we see that the increased complexity of the model allowed for a greater number of VI topics and phenomena to be explored.

The processes of VI may be described by partial differential equations (PDEs). Unfortunately, there rarely are any analytical solutions to these (except in the most simple cases) and numerical methods are required to find approximate solutions. One of the most powerful numerical methods for solving PDEs is the finite element method, which not only allows us to find solutions to PDEs but does so for complex three-dimensional geometries.

The purposes of this thesis is not to explain the FEM in any great detail, but there are many great resources available for those who are interested in learning more. There are however, two things that are important to know what makes the FEM unique.

The first is the FEM divides up a complicated geometry into smaller *finite elements*, hence its name. Which elements exactly depend on the dimensionality of the model and the specific problem that one wish to solve. Three-dimensional geometries are usually represented by tetrahedral and two-dimensional ones by triangles.

The second is that the solution to a PDE may be represented by a series of *basis*

Figure 1.1: Example of a simple conceptual site model of a vapor intrusion site.

*functions* with an associated function *coefficient*.

$$u \approx \sum_i u_i \psi_i \quad (1.1)$$

The development of the three-dimensional finite element vapor intrusion models begin with a conceptual site model (CSM) of a VI site. In general when one develops models, it is best in the beginning to keep the model as simple as possible, and not to add overly complex features or excessive physics. As such, we begin with a very simple CSM which may be seen in Figure 1.1.

This CSM features a residential building with a 10 by 10 m footprint, with a concrete foundation one meter below ground-surface (bgs). Along the perimeter of foundation there is a one cm wide breach, through the subsurface contaminants enter the house. Three meters below the foundation, there is a contaminated groundwater source, from which contaminants vapor continuously evaporate. The house is assumed to be depressurized relative to the atmosphere which creates a pressure gradient, allowing air to be pulled through the ground-surface, soil, and into the house - carrying some contaminants with it. The indoor air is also exchanged at a constant rate with the outside environment, which is the only way the contaminant leave the house. For simplicity we also assume that the soil is completely homogenous.

To implement this CSM as a finite-element model several steps must be followed.

1. Construct a model geometry (domain).
2. Assign relevant partial differential equations (PDEs) and boundary conditions (BCs) that describe the physics.
3. Mesh the geometry.
4. Configure and choose solvers.
5. Post-processing.

Each step will be carefully explained, beginning with the construction of the domain.

## 1.2 The Indoor Environment

The indoor air space is perhaps the most important part of modeling VI, as the goal of these models ultimately is to predict indoor exposure given external factors. One could therefore assume that most of the effort in modeling VI should be spent to accurately represent the interior. This would be very impractical however, as building interiors are so diverse. Even if one would spend the time to model an interior, this would dramatically increase the number of mesh elements required to solve the model. Additionally, the air flow inside the building must be calculated, and even using a simplified version of Navier-Stokes, like Reynolds Averaged Navier-Stokes, the computational cost would be significant.

The indoor air space is implicitly modeled and the part of the model geometry that would be the house is instead an empty space.

as a continuously stirred tank reactor (CSTR), and paradoxically becomes the simplest component of the VI model.

The fundamental assumption of a CSTR is that any contaminant or chemical species entering, or inside the indoor air space (control volume), is perfectly mixed, i.e. there are no spatial gradients, and is given by (1.2)

$$V \frac{\partial c}{\partial t} = n - V A_e c + R \quad (1.2)$$

Here  $n$  is the contaminant entry rate into the building.  $A_e$  is the air exchange rate, which determines the which portion of the indoor air is exchanged for a given time period, e.g. if  $A_e$  is 0.5 per hour, half of the indoor air is exchanged over one hour.  $R$  can be the generation of contaminant vapor from an indoor source or sorption, but is usually assumed to be zero.

## 1.3 Water Flow in Unsaturated Porous Media

Richard's law etc

### 1.3.1 Soil-Water Potential

### 1.3.2 Soil-Water Retention Curve

The distribution of soil moisture in the soil matrix has profound implications for the advective and diffusive transport of contaminants. Soil has a limited amount of pore volume available for contaminant transport, and the presence of water restricts this further; decreasing permeability of the soil and subsequently reduces air flow. Diffusivity of the contaminant will also be retarded by the water. The contaminant will dissolve into and evaporate from water and the transport will partially occur through water. Liquid diffusion coefficients are usually around four orders of magnitude smaller than in air.

The soil moisture content of soils can be estimated in many ways, but two common approaches is to use the analytical formulas of *van Genuchten* or *Brooks and Corey*. Both of these formulas give the soil moisture content as a function of the fluid pressure head,  $H_p$ . By definition, when the pressure head is equal to or greater than zero,  $H_p \geq 0$ , the soil is assumed to be 100% saturated with the fluid. In this work, *van Genuchten's* formula is used.

The soil moisture content,  $\theta$  is given by.

$$\theta = \begin{cases} \theta_r + \text{Se}(\theta_s - \theta_r) & H_p < 0 \\ \theta_s & H_p \geq 0 \end{cases} \quad (1.3)$$

The saturation is given by.

$$\text{Se} = \begin{cases} \frac{1}{(1+|\alpha H_p|^m)^m} & H_p < 0 \\ 1 & H_p \geq 0 \end{cases} \quad (1.4)$$

$$C_m = \begin{cases} \frac{\alpha m}{1-m}(\theta_s - \theta_r) \text{Se}^{\frac{1}{m}} (1 - \text{Se}^{\frac{1}{m}})^m & H_p < 0 \\ 0 & H_p \geq 0 \end{cases} \quad (1.5)$$

$$k_r = \begin{cases} \text{Se}^l [1 - (1 - \text{Se}^{\frac{1}{m}})]^2 & H_p < 0 \\ 0 & H_p \geq 0 \end{cases} \quad (1.6)$$

## 1.4 Vapor Transport in Unsaturated Porous Media

Vapor transport in porous media is described by *Darcy's Law*. The vapor velocity depends on the pressure gradient in the soil, is proportional to the permeability of the soil matrix, and is inversely proportional to the viscosity of the fluid.

$$\vec{u} = -\frac{\kappa}{\mu} \nabla p \quad (1.7)$$

For Darcy's Law to be valid, two assumptions must be fulfilled:

1. The fluid must be in the laminar regime, typically  $\text{Re} < 1$ .
2. The soil matrix must be saturated with the fluid.

In VI-modeling, the first assumption is fulfilled, but the second is not. Most of the contaminant vapor transport takes place in the partially saturated vadose zone and thus, (1.7) needs modification.

In partially saturated soils, a varying portion of the soil pores are available for vapor transport, with the rest being occupied by water, affecting the effective permeability of the soil. To model this, a relative permeability property,  $k_r$ , is introduced:

$$\kappa_{\text{eff}} = k_r \kappa_s \quad (1.8)$$

$k_r$  is a dimensionless parameter that varies between 0 and 1, and  $\kappa_s$  is the saturated, or simply the soil matrix permeability.

This gives the modified Darcy's Law used in VI-modeling:

$$\vec{u} = -\frac{k_r \kappa_s}{\mu} \nabla p \quad (1.9)$$

## 1.5 Mass Transport in Unsaturated Porous Media

Advective-diffusion equation

$$\frac{\partial}{\partial t}(\theta c_i) + \frac{\partial}{\partial t}(\rho_b c_{P,i}) + \frac{\partial}{\partial t}(a_v c_{G,i}) + \vec{u} \cdot \nabla c_i = \nabla \cdot [(D_{D,i} + D_{eff,i}) \nabla c_i] + R_i + S_i \quad (1.10)$$

## 1.6 References