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 to learn 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 linear com-

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

bination of a series of *basis functions* with an associated function *coefficient*.

$$u \approx \sum_i u_i \psi_i \tag{1.1}$$

where u is the solution to the PDE, u_i is the coefficient associated with the basis function ψ_i. This approximation allows the PDE to be discretized into a matrix and the u_i coefficients are solved for. Any function may serve as a *basis function*, but typically a simple one is chosen (for simpler computation) like a linear hat function or low-degree polynomial. In certain applications, some basis functions perform better than other, but in most cases linear hat functions or second-degree polynomials are preferable.

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 Geometry

Designing the model geometry is the first step to creating a 3D FEM model. It is one of the most important steps, as the geometry will dictate the model accuracy and astute geometry design will help save computational resources. When designing a geometry the FEM user should have the following goals in mind:

1. Represent the model geometry as accurately as possible.

2. Avoid unnecessarily fine details.

3. Try to leverage symmetry to reduce geometry size.

The first point is somewhat self-explanatory, as we obviously want to create a model geometry that is as similar to what we want to model as possible. The second points can at times run counter to the first and may be more self-evident once meshing is more thoroughly discussed. Tiny details often require a significant number of mesh elements to be fully resolved, disproportionally adding to the total number of mesh element, and may significantly increase computational costs. This is when the skill and judgement of the modeler comes in - choosing which details to omit and which to keep. As a rule-of-thumb one should for the most part try to only model parts of the geometry that is of significant value to the question that one wants answered. In VI modeling, one such obvious area is the crack or breach in the foundation through which contaminant vapors enter the structure, resolving this tiny part of the geometry is of great importance.

The third point is something that the modeler should always be on the lookout for when designing a model geometry - if there are any planes of symmetry in the geometry. Finding a plane of symmetry allows us to reduce the size of the model and save significantly computational costs. A simple example of this is one wants to model a pipe with static mixers inside, then only a sector of the cylinder's face may be necessary to be modeled. Using the simple CSM described by Figure 1.1 only a quarter of the house and surrounding property is necessary to be explicitly modeled, cutting the number of required mesh elements down to just a quarter of what would otherwise be necessary - a huge computational saving!

1.2.1 Geometric Components

Model geometries are typically designed in some sort of computer assisted design (CAD) software. The exact tools and techniques available to the modeler will vary from software to software, with some featuring import options for real-world scanned 3D geometries to combining simple geometric objects through various Boolean operations. The software we use, COMSOL, uses primarily the latter method of combining simple objects to form more complicated ones but more capabilities may be purchased.

To create a model geometry of the CSM in Figure 1.1, only a few simple geometric objects and Boolean operations are required - two cuboids, two rectangles, one Boolean difference operation, and one Boolean join operation. The following steps are needed:

1. Create a block or cuboid that is 15 meter wide and long, and with a height of 4 meter.

2. Create another block that is 5 meter wide and long, with a height of 1 meter.

3. Place the second block 3 meter above zero, so that the top surfaces of the two blocks intersect.

4. Perform a difference operation, removing the smaller block from the first one.

At this point you will see that a quarter soil domain has been created, with an empty space that will represent a house with a foundation slab located 1 meter below ground-surface.

The foundation crack will be modeled as a 1 centimeter wide strip that spans the perimeter of the surface that represents the house foundation. To create the crack do the following:

1. Create a work plane 3 meter above zero.
2. Create two rectangles that are as long as the foundation, with a width of 1 centimeter, rotating one 90 degrees, and making sure that they are place along the foundation perimeter.
3. Join the two rectangles using a Boolean union (do not keep the interior boundaries).

Now that the foundation crack is generated, we have designed a model geometry of the simple CSM and the complete geometry may be seen in Figure 1.2. The next step is to choose and setup the appropriate physics required to model VI, beginning with modeling the indoor environment.

Figure 1.2: The complete geometry of the CSM described in Figure 1.1.

In the appendix, there will be further explanations for additions to the model geometry that will be necessary for modeling various VI scenarios.

1.3 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)

$$V\frac{\partial c}{\partial t} = n - VA_e c + R \tag{1.2}$$

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.

1.4 Water Flow in Unsaturated Porous Media

Richard's law etc

1.4.1 Soil-Water Potential

1.4.2 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, θ is given by.

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

The saturation is given by.

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

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

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

1.5 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.

$$\vec{u} = -\frac{\kappa}{\mu}\nabla p \tag{1.7}$$

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

1. The fluid must be in the laminar regime, typically 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:

$$\kappa_{\text{eff}} = k_r \kappa_s \tag{1.8}$$

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

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

$$\vec{u} = -\frac{k_r \kappa_s}{\mu}\nabla p \tag{1.9}$$

1.6 Mass Transport in Unsaturated Porous Media

Advective-diffusion equation

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

1.7 Meshing

1.8 Solver Configuration

1.9 References