

# Vapor Intrusion: Modeling of Dynamic Processes

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## Abstract

Vapor intrusion (VI) investigations, the effort to determine the exposure and associated human health-risk at a VI impacted building, are often complicated by significant spatial and temporal variability in VI. Over the years there have been efforts to develop new techniques and methodologies that aim to reduce the issues associated with these variabilities; simplifying and improving the robustness of VI site investigations. The development of the controlled pressure method (CPM), where the pressurization of a building is controlled to increase or decrease contaminant entry into the building, is one such example. Another approach is to use indicators, tracers, and surrogates (ITS) to help guide when to conduct site investigations, ideally increasing the likelihood of determining the higher indoor contaminant concentrations.

Both of these approaches rely on a quasi-deterministic relationship between some external variable, such as building pressurization, and indoor contaminant concentration. However, site-specific conditions can give rise to very different responses to such an external variable, and to effectively use CPM or ITS, a better mechanistic understanding of contaminant transport and exposure are needed.

In this thesis, we develop three-dimensional finite element models of VI impacted buildings from a first principles perspective. These models combined with analysis of field data from VI sites, allows us to explore the physical mechanisms that drive VI. By considering the dominant contaminant transport mechanism at a site, e.g. if advective or diffusive transport dominates, we can explain why a change in building pressurization can lead to such differences in contaminant concentration at different sites. We can also better understand how various factors in VI contribute to the overall variability.

By classifying the dominant contaminant transport mechanism at a site, we can more effectively anticipate how a particular site will respond to some external stimuli. This will in turn reduce the effort required to, and increase the robustness of the techniques used determine the relevant human exposure at a VI site.

# Dedication

To mum and dad

# Declaration

I declare that..

# Acknowledgements

I want to thank...

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# Chapter 1

## Introduction

### 1.1 Indoor Air Quality Perspective

Concerns about air quality are as old as civilization itself, ranging from beliefs that disease is caused by bad air - a *miasma*, to more recent concerns about exposure to combustion particulates. Since industrialization the number of potential hazardous pollutants has increased significantly, followed by increased concerns about air quality. At the same time, people now spend more time indoors now than ever before, with Americans spending up to 90% of their waking time indoors[?]. This change in human habitation has put a special emphasis on indoor air quality.

Some early scientific inquiries into indoor air quality focused on pollutant sources that were generated in the home, such as heating and cooking systems. Increased levels of carbon monoxide, sulfur dioxide, and various nitrous oxides could be detected due to these systems[?]. These types of pollutants are still relevant today, but of particular concern in developing countries[?].

Some indoor air pollutants may be emitted from building materials, such as asbestos from older types of insulation, or formaldehyde from pressed-wood products, and various petroleum or chlorinated compounds may be emitted from common household product. Molds are another common indoor quality concern[?].

Indoor air quality may be significantly affected by external contaminant sources as well, with Radon being perhaps one of the most well-known cases of this. Radon is a radioactive gas produced by the natural decay of Uranium 238, which is commonly found in many rocks and minerals. These in turn are often found in the soil or bedrock and the Radon gas enter the overlying buildings, exposing the inhabitants.

### 1.2 Vapor Intrusion

A recent addition to the myriad of indoor air quality concerns is vapor intrusion (VI) - a process that is similar to Radon intrusion. As with Radon intrusion, VI contaminants are typically originate from underneath a building, migrate through the soil, entering it, and exposing the inhabitants. VI is different from Radon intrusion because it is more broad and general; the contaminant sources are usually of anthropogenic origin, and not limited to the soil. As such, Radon intrusion can be thought of as a subset of VI, but they are typically considered separately. In VI, the primary contaminants of concern are chlorinated solvents, e.g. trichloroethylene (TCE),

tetrachlorethylene (PCE), vinyl chloride, chloroform, and organic compounds, e.g. benzene.

The prototypical VI scenario is one where groundwater has been contaminated with one or many of these contaminants. Contaminant vapors evaporate from the groundwater, and are transported through the soil into the overlying buildings through small cracks and breaches in the foundation. While this simple example is helpful for gaining a rudimentary understanding of VI, it fails to capture much of the complexities of an actual VI site.

Determining if vapor intrusion occurs at a house or structure is often difficult. One might be tempted to believe that taking an air sample inside the house would be sufficient, i.e. that vapor contaminant concentrations is over some threshold in the house is proof of VI; absence of contaminant vapors is proof of no VI. The reality is that indoor air samples can be problematic for a few reasons. Due to their distributive nature, the residents or owners of the structure may be unwilling to let indoor samples to be taken. Indoor air samples are also susceptible to false positives and negatives.

Many common consumer products contain the same contaminants that is often of concern in VI. The presence of these contaminants in a house is thus not necessarily proof of VI but rather a line-of-evidence. Great care should be and is taken to remove any potential indoor contaminant sources before any VI investigation can begin (contributing to the distributive nature of these investigations).

There can be significant temporal variability of indoor contaminant concentrations and some sites may have "active" and "inactive" periods, thus the absence of indoor contaminant is not proof that VI is not occurring, but yet another a line-of-evidence. This temporal variability occurs on different time-scales as mean indoor contaminant concentrations often fluctuate across seasons, and may even significantly vary across weeks, days, or even within a day.

Another approach might be to collect groundwater and/or soil-gas samples, but this also has it's inherent issues as well. The presence of contaminant in the groundwater or surrounding soil-gas (even if found right underneath the foundation) is evidence that VI occurs. Likewise, the absence or low concentration of contaminants may only indicate that there is significant spatial variability in contaminant concentration or that the source has not been found (hidden preferential pathways may especially be issues in the latter case). The result of these samples is the same as indoor samples, they may only be used as a line-of-evidence for VI.

The combination of these line-of-evidence are usually required to prove that VI occurs; the presence of contaminant in the groundwater, in the soil-gas underneath the structure, and finally inside the structure would be good evidence that VI occurs. This multiple line-of-evidence (MLE) approach is necessary when conducting VI investigations and is recommended by the United States Environmental Protection Agency (EPA).

## 1.3 Mathematical Modeling of Vapor Intrusion

With the growing need to understand and more importantly - predict exposure to contaminant vapors at VI sites the range of available tools has subsequently increased. One such important tool has been the development of mathematical models that, based on the complex factors and processes that govern VI, allow



deterministic predictions to be made. Over time mathematical modeling of VI has become an important and intrinsic part of VI investigations, both as a MLE and as an investigative tool.

VI models have a wide range of potential applications, such as:

- Designing experiments and interpretation of results.
- Guiding site investigations and make sense of the findings.
- Estimating indoor air quality in advance of construction.
- Designing mitigation systems.

This is not an exhaustive list, and models are more or less widely used in these applications. As models become more advanced and validation continues, their capabilities will likewise increase.

Johnson and Ettinger developed one of the first mathematical models of VI[?], based on earlier work by Nazaroff who developed a model to predict Radon intrusion[?]. The goal of these models was to provide heuristic screening level calculations, allowing the user to gain a rough idea of the degree of VI by specifying, e.g. soil type, building pressurization, air exchange rate, and groundwater contaminant concentration. The Johnson and Ettinger model is to date one of the most commonly used VI models and was implemented in an Excel spreadsheet and distributed on the EPA's website.

Over time these models have become more advanced, moving from the one-dimensional Johnson and Ettinger model to modeling VI in two or three dimensions, incorporating more advanced physics, and allowing time-dependent simulations to be run. This advanced modeling necessitated the use of numerical methods to be solvable. One of the more advanced and general examples of these models are the those developed by Bozkurt et al.[?], Pennell et al.[?], Shen et al.[?], Yao et al.[?], and Ström et al.[?], which utilize the finite element method to simulate VI. A more detailed review of VI models will be presented in Chapter ??.

## 1.4 Research Motivation

Recently significant effort has been spent on studying VI. Some very notable examples of this are two VI impacted residential homes that were purchased for the sole purpose of conducting highly detailed and long-term studies of VI at these sites. A key motivator for these studies was to in particular study and understand the temporal variability of VI that has been found at many other sites.

The first was a house located near Hill AFB in Utah, which was a co-financed project between Arizona State University (ASU) and the EPA. The principal investigators at the site was a research team lead by Dr. Paul Johnson from ASU and therefore this site is hereafter referred to as simply the ASU house. Detailed descriptions of the experimental setup at this house may be found in [?]. Suffice to say that this was a highly detailed study where high-frequency indoor air samples of various contaminants were collected in different parts of the house as well as soil-gas and groundwater samples in different locations and depths. Simultaneously tracer gas studies were continuously conducted to measure the building air exchange rate.

Pressure differences between the indoor and outdoor as well as several meteorological metrics were also collected.

The second house was located in Indianapolis, Indiana, and was purchased and invested solely by the EPA. Similar to the ASU house, this house was outfitted with multiple probes for sampling indoor, groundwater, and soil-gas contaminant concentration at various locations and at high frequency. Likewise a pressure differences and meteorological metrics were measured, amongst other things. These sites present a rich and invaluable dataset for understanding VI.

From the onset of the studies at the EPA and ASU houses, it was believed that the VI source was the contaminated groundwater underneath these structures. Later it was discovered that these sites both were impacted by what is now known as preferential pathways. A preferential pathway is a term that refers to a process or feature that facilitates the transport of vapor contaminants from a source into the building of concern. An example of this is subsurface pipe networks such as sewers, land drain, or other piping.

At the ASU house, the preferential pathway was a sewer connected land drain that exited underneath the house (with the purpose of draining excess water underneath)[?]. For the EPA house, a leaky, house connected sewer pipe was the preferential pathway[?]. In both of these cases it seems like the main sewer line had been infiltrated by contaminated groundwater and through the piping, a preferential pathway for the vapor contaminant was established. Both of these preferential pathways mainly introduced vapor contaminants in the near subsurface underneath, and were subsequently transported into the houses, but other studies show that contaminant vapors may be introduced from sewers through broken plumbing fixtures[?, ?].

The ASU house study demonstrated the significant role preferential pathways can play in VI, and their discovery is an important part of a VI investigation. But as of yet it is fairly poorly understood how and when a preferential pathway may play a significant role or not. By contrast to the ASU house, the significance of the preferential pathway at the EPA house is not as clear, and seem to have had quite different effects of the two respective sites. A lesson learnt from these two sites is that finding these preferential pathways is not always a trivial matter, and research into if and when preferential pathways matter can help by narrowing down the search for them.

One significant effect of the preferential pathway at the ASU house was that it greatly enhanced the advective potential at the site, making the house much more sensitive to changes in pressurization[?, ?, ?]. This same strong association between the VI potential and building pressurization was not observed at the EPA house however, even with a preferential pathway present (again showing that their effect can vary significantly). Another site in San Diego, California, however, again showed very significant correlation between VI potential and building pressurization[?].

These varied associations between VI potential and building pressurization are not very well understood. Typically the building pressurization fluctuate across the span of a day and often exhibit seasonal trends - making pressurization a prime candidate in driving much of the temporal variability of VI. Therefore, an examination of which site characteristic less or increase a building's sensitivity to pressurization is necessary to bridge this gap.

Building pressurization is not the only factor that exhibit seasonal trends; temperature, air exchange rate, rainfall, snow coverage, and groundwater depth all

vary across time and often (depending on a site's climate) exhibit seasonal trends. Understanding these trends, and how they impact VI are crucial for collecting representative and dependable samples at a site. E.g. should one immediately collect indoor air samples after rain? Or is it more prudent to wait a few days? Or weeks?

Many VI contaminants have the potential to sorb onto various common indoor materials and soils. However, so far it is relatively unknown how sorption processes affects VI as a whole.

## 1.5 Research Objective

This research's broad aim is to improve our understanding of the complex fate and transport of VI contaminants, with a particular focus on the dynamic processes that drive the temporal variability in VI. The ultimate goal is to reduce the uncertainty in VI investigations, and to make these easier and cheaper to conduct. To achieve this we mathematically describe the processes that govern the fate and transport of VI from a first principles approach. These are implemented and numerically solved using a finite-element method (FEM) solver package - COMSOL Multiphysics, which generate deterministic models of VI scenarios. By combining these models with statistical analysis of high-resolution datasets from the two well-studied VI sites, the ASU house and the EPA house, we gain an opportunity to explore the dynamic VI processes.

These models and analysis are applied to understand the role that pressure fluctuations have on determining temporal variability, and how the preferential pathway discovered at the ASU house enhanced this influence. The influence the preferential pathway had at the EPA house is likewise investigated. Seasonal driving forces, and in particular how temperature and wind affect building pressurization and air exchange rate, and how these can be used to explain much of the long-term seasonal changes in VI potential can be explained by these. We also explore the role that contaminant sorption, both onto soil and various indoor materials, have on the transient response to pressure changes. Lastly, these findings are explored in relation to the application of the controlled pressure method (CPM), and the significance of their impact on effective use of CPM.

## 1.6 Outline

The thesis is divided up into X chapters...

## Chapter 2

# Developing Vapor Intrusion Models

## ***Abstract***

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Vapor intrusion (VI) investigations, the effort to determine the exposure and associated human health-risk at a VI impacted building, are often complicated by significant spatial and temporal variability in VI. Over the years there have been efforts to develop new techniques and methodologies that aim to reduce the issues associated with these variabilities; simplifying and improving the robustness of VI site investigations. The development of the controlled pressure method (CPM), where the pressurization of a building is controlled to increase or decrease contaminant entry into the building, is one such example. Another approach is to use indicators, tracers, and surrogates (ITS) to help guide when to conduct site investigations, ideally increasing the likelihood of determining the higher indoor contaminant concentrations.

Both of these approaches rely on a quasi-deterministic relationship between some external variable, such as building pressurization, and indoor contaminant concentration. However, site-specific conditions can give rise to very different responses to such an external variable, and to effectively use CPM or ITS, a better mechanistic understanding of contaminant transport and exposure are needed.

In this thesis, we develop three-dimensional finite element models of VI impacted buildings from a first principles perspective. These models combined with analysis of field data from VI sites, allows us to explore the physical mechanisms that drive VI. By considering the dominant contaminant transport mechanism at a site, e.g. if advective or diffusive transport dominates, we can explain why a change in building pressurization can lead to such differences in contaminant concentration at different sites. We can also better understand how various factors in VI contribute to the overall variability.

By classifying the dominant contaminant transport mechanism at a site, we can more effectively anticipate how a particular site will respond to some external stimuli. This will in turn reduce the effort required to, and increase the robustness of the techniques used determine the relevant human exposure at a VI site.



## 2.1 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 combination of a series of *basis functions* with an associated function *coefficient*.

$$u \approx \sum_i u_i \psi_i \quad (2.1)$$

where  $u$  is the solution to the PDE,  $u_i$  is the coefficient associated with the basis function  $\psi_i$ . 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 2.1.



Figure 2.1: Example of a simple conceptual site model of a vapor intrusion site.

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.

## 2.2 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 2.1 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!

### 2.2.1 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 2.1, 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 attentive reader will now of course notice that an entire house is missing from the model geometry. This is intentional, as explicitly modeling the interior of a building is too impractical for two primarily two reasons. First is that house interiors are simply too diverse for any explicit model to truly be representative in any general sense, not to mention how laborious it would be to create such a model interior. Secondly, the computational costs required to solve the air flow inside (necessary for accurate representation of contaminant transport/distribution inside) would be significant. The Navier-Stokes equation would need to be solved, and even using one of the simpler versions of it (large eddy simulation or Reynold's

averaged) would impose a significant cost at questionable gain. Therefore the indoor air is modeled implicitly, which will be covered in detailed in section 2.3.

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 2.2. The next step is to choose and setup the appropriate physics required to model VI, beginning with modeling the indoor environment.

Figure 2.2: The complete geometry of the CSM described in Figure 2.1.

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

## 2.3 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 large eddy simulation or Reynolds averaged, the computational cost would be significant.

To overcome this, the indoor environment is instead modeled as a continuously stirred tank reactor (CSTR). 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 the ordinary differential equation (ODE) (2.2).

$$V \frac{\partial c_{\text{in}}}{\partial t} = n - V A_e c + R \quad (2.2)$$

Here  $c_{\text{in}}$  is the indoor air contaminant concentration in  $\text{mol}/\text{m}^3$ ;  $n$  is the contaminant entry rate into the building in  $\text{mol}/\text{s}$ ;  $A_e$  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 used to

simulate sorption of contaminants vapor in the indoor environment, and if this is not of interest it can simply be set to zero; Finally,  $V$  is the volume of the building interior in  $\text{m}^3$ . Typically this is set to only reflect the volume of the floor or rooms on top of the building foundation. Since the indoor environment is does not explicitly "belong" anywhere in the COMSOL model, it is modeled using the "Global ODE" interface.

### 2.3.1 Contaminant Entry

The most important component of (2.2) is of course determining the contaminant entry rate  $n$ , and is the most challenging portion of the modeling effort. The contaminant entry rate has two transport components, advective and diffusive which depends on three factors:

1. The velocity of the contaminant vapors entering or exiting the structure though the foundation crack.
2. The contaminant vapor concentration in the near vicinity of the foundation crack.
3. The indoor air contaminant concentration itself.

**Advective Transport** The advective transport due to the bulk motion of the contaminant vapors and the flux is given by (2.3).

$$j_{\text{adv}} = \vec{u}c \quad (2.3)$$

The bulk motion of the contaminant vapor is given by the vector quantity  $\vec{u}$  in  $\text{m/s}$  and  $c$  is the contaminant vapor concentration.

**Diffusive Transport** The diffusive transport is due to a concentration gradient, modified by a diffusion coefficient, and is given by Fick's law (2.4)

$$j_{\text{diff}} = \nabla \cdot (D\nabla c) \quad (2.4)$$

Where  $\nabla$  is the del operator and  $D$  is the diffusion coefficient in  $\text{m}^2/\text{s}$ . In this formulation,  $D$  does not have to be a constant and can depend on the coordinate or concentration.

The implication of this is that (2.2) has to be coupled with the equations that describe the contaminant concentration in the soil as their solutions are dependent on each other. How this is achieved will be covered in section 2.4.3 when discussing boundary conditions.

### 2.3.2 Air Exchange Rate

The air exchange rate,  $A_e$  is the parameter that determines the rate at which the contaminant vapors leave the indoor environment. Air infiltrate and exfiltrate through a building primarily via two mechanisms

1. Through breaches and orifices in the building envelope, e.g. windows, slits, or other small opening.

## 2. Passive or active ventilation.

With the exception of active ventilation, where air is mechanically forced to enter or exit the building, the driving force for the in-/exfiltration is driven by a pressure gradient between the indoor and outdoor environment,  $p_{\text{in/out}}$ . These pressure gradient are primarily due to differences in indoor and outdoor temperatures and to wind striking the building and quantifying these pressures differences is covered in section 2.3.3.

**Quantifying Air Exchange Rate** While air exchange rate is largely driven by the indoor and outdoor pressure difference, it is not possible to quantify their relationship for the range of pressures that a building is naturally pressurized; there is too much uncertainty. In Figure 2.3 a two-dimensional kernel density estimation (a way to estimate probability distributions[?]) of indoor/outdoor pressure and air exchange rate from the well-studied ASU house shows the relationship between these[?]. The a darker color signifies are closer association or overlap but by the lack of any visual trends (it is all a blob) combined with a Pearson's  $r$  value of  $x$ , it is apparent that there is no real correlation between them exist.

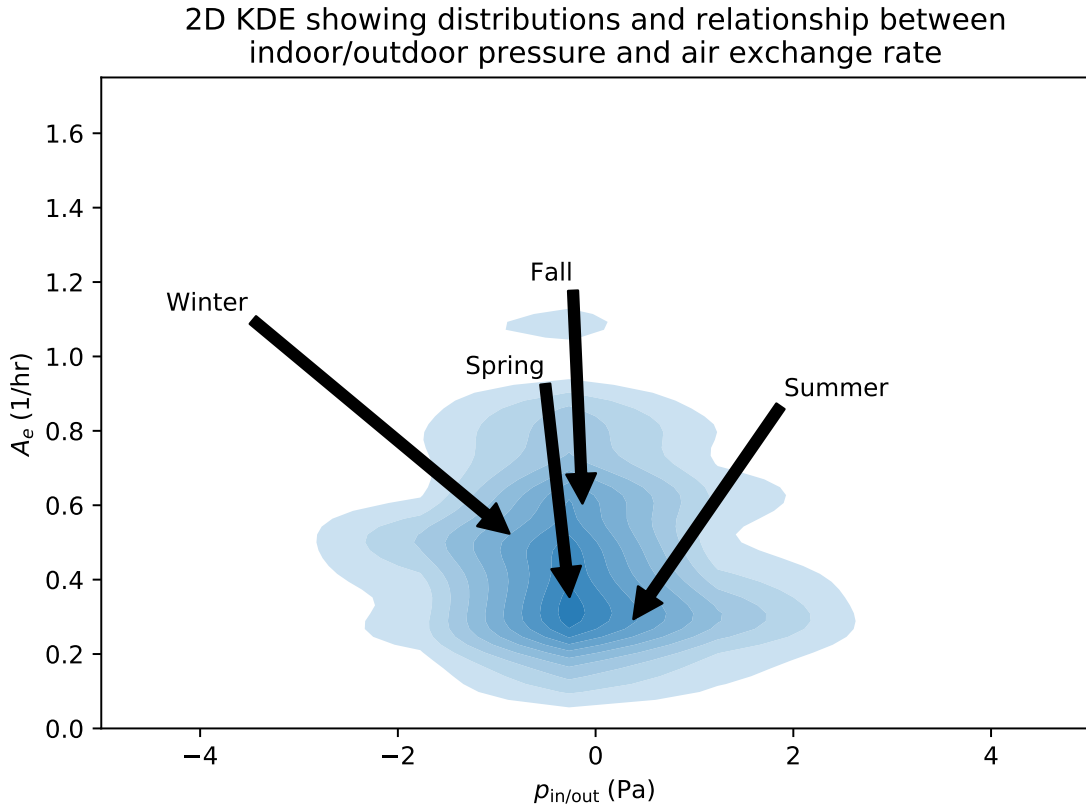


Figure 2.3: Distributions of indoor pressurization and air exchange rate and their relationships; seasonal medians indicated by arrows.

**Building Leakage Curves** It is possible to quantify air exchange rate if a building is sufficiently pressurized through building leakage curves.

### 2.3.3 Quantifying Pressure Difference Induction

**Wind Effects** As the wind strikes a surface its velocity falls to zero, and the change in momentum is directly proportional to the change in pressure:

$$\Delta P = \frac{1}{2} \rho_{\text{air}} u_{\text{wind}}^2 \quad (2.5)$$

where  $\Delta P$  is the change in pressure;  $\rho_{\text{air}}$  is the air density; and  $u_{\text{wind}}$  is the wind speed.

In reality however, the pressure drop is not quite so straightforward due to several factors, e.g. building envelope contains various structures and may be shielded by other objects. To account for this, a drag or pressure coefficient  $C_d$  is introduced to moderate the pressure drop:

$$\Delta P = C_d \frac{1}{2} \rho_{\text{air}} u_{\text{wind}}^2 \quad (2.6)$$

This coefficient is usually determined empirically from e.g. wind tunnel studies.

**Temperature Effects** The pressure of any fluid under the influence of gravity varies with elevation and the density of the fluid determines the magnitude of this pressure. Air is a compressible fluid and its density depends on its temperature. Therefore, if you separate two air masses between a wall, with each at a difference temperature, a pressure difference across the wall be induced, i.e. the *stack effect*.

Assuming the ideal gas law applies and that the temperature on either side is constant then

$$P = P_0 \exp \left( \frac{-M_{\text{air}} g z}{RT} \right) \quad (2.7)$$

determines the pressure variation across the wall. Where  $P$  is the pressure;  $P_0$  the reference pressure ( $z = 0$ );  $M_{\text{air}}$  is the molar weight of air;  $z$  is the elevation;  $g$  is the acceleration due to gravity;  $R$  is the gas constant; and  $T$  is the temperature.

This can be further simplified by defining  $z_0$  which is the height at which the pressure on both sides of the wall are equal, i.e.  $P_0$ . The pressure variation on either side can now be expressed in terms of distance from  $z_0$ ,  $z - z_0$ . Assuming that the interior and exterior has a constant temperature of  $T_i$  and  $T_o$  respectively, the difference in pressure between the two sides along the wall is

$$\Delta P = P_0 \left[ \exp \left( \frac{-M_{\text{air}} g (z - z_0)}{RT_i} \right) - \exp \left( \frac{-M_{\text{air}} g (z - z_0)}{RT_o} \right) \right] \quad (2.8)$$

Using that  $e^{-x} = 1 - x$  for  $x \ll 1$  the pressure difference can be expressed as

$$\Delta P = \alpha \left( \frac{1}{T_o} - \frac{1}{T_i} \right) (z - z_0) \quad (2.9)$$

where  $\alpha = \frac{P_0 M_{\text{air}} g}{R} \approx 3454 \frac{\text{Pa} \cdot \text{K}}{\text{m}} \text{Pa}$ . Here a negative pressure difference,  $\Delta P < 0$ , indicates an inward flow.

**Other Effects** Other factors also contribute to the pressure difference between the interior and exterior. Some examples of these are various combustion processes (fireplaces), ventilation fans, or even human factors such as opening and closing doors or windows.

### 2.3.4 Indoor Sources

There are two types of indoor sources in VI. The first are various products and items that contain the contaminant of concern and continuously emit these. Some examples of these may be various cleaning products, degreasers, gasoline tanks, or even recently dry-cleaned clothing. These are usually not considered to be part of the VI phenomena themselves (even though they can pose health risks) but rather items that need to be removed in a VI investigation to prevent false positives.

The second type are the walls, furniture, objects, or features inside the interior that sorb the contaminant vapors. While these are not *sources* in the strict sense, they may never the less contribute to the overall contaminant exposure. How significant these secondary types of indoor sources are largely depend on the material. Some, such as cinderblock concrete have a very large capacity to hold contaminant vapors while others such as fabrics do not.

**Sorption Processes** Modeling the secondary type indoor sources (sorption onto materials) can be done with a simple equilibrium reaction:

$$c^* \xrightleftharpoons[k_2]{k_1} c_{in} \quad (2.10)$$

## 2.4 Soil Physics Governing Vapor Intrusion

The soil surrounding the structure in our VI model is, unlike the indoor environment, modeled explicitly. In this section we will walk through each physics, the associated governing equation, and boundary conditions required to model the contaminant transport in soil. The following physics and governing equations will be covered:

1. Water flow in unsaturated porous media
2. Vapor transport in unsaturated porous media
3. Mass transport in partially saturated medium

In addition to these, the modeling of the temperature distribution in the soil is covered in Appendix .

The vapor contaminant transport through the soil in VI occurs through the vadose zone - soil that is partially filled with water, giving a three-phase transport system. This partial water content has profound effects on both advective and diffusive transport and modeling the water content is achieved via *Richard's equation*. Since the vapor and mass transport in the soil are so dependent on the soil water content, it is covered first in the following section 2.4.1.

The mass transport in the soil has both an advective and diffusive component. The advective transport in the soil is dictated by the vapor flow in the soil which is described by *Darcy's Law* making it the next logical step to cover in section 2.4.2. The diffusive transport depends on the contaminant vapor concentration itself and accurately modeling this requires coupling with all of the physics discussed so far (including the indoor environment). Therefore the mass transport physics, governed by the *advection-diffusion equation* will be covered last in section 2.4.3.

### 2.4.1 Water Flow in Unsaturated Porous Media

The vadose zone or unsaturated zone is a region of soil between the top of the ground surface and the water table. In the vadose zone there are two fluid phases, one gas and the other liquid (usually air and water) inside the porous soil matrix giving a three phase system; only one fluid phase (gas or liquid) exist in the saturated zone. As a result, the transport properties in the vadose zone differ from that in a zone saturated where there are only two phases present - water and soil.

#### Soil-Water Potential and Retention Curve

The driving force, or soil-water potential, for the filling and draining of pore water in soils are due to a pressure and a gravitational potential and given by  $\phi$ . This phenomena is called *capillary potential* or *matrix potential*,  $\psi$ , which depends on the volumetric water content  $\theta$  in the soil.

Over the years, there has been a few attempts of characterizing the relationship between soil moisture content  $\theta$  and soil water potential  $\phi$  - a so-called soil water retention curve. Two common relationships have been proposed by Brooks and Corey in 1966[?], and another by van Genuchten in 1980[?]. Both of these approaches are semi-empirical and each is a function of the soil water potential with several fitting parameters. These parameters are specific to each soil type and usually are derived from laboratory experiments. In our VI models we chose to use the van Genuchten formulation for the simple reason that these have been historically used in VI modeling and the associated parameters are well-known for a variety of soils.

In the van Genuchten formulation that we use, pressure head  $H_p = \frac{p}{\rho g}$  is used as the dependent variable instead of the soil water potential  $\psi$ . Here  $p$  is the fluid pressure;  $\rho$  the fluid density; and  $g$  is the acceleration of gravity. The fluid is here water. By definition the soil matrix is saturated with fluid when the pressure head is zero  $H_p = 0$  and variably saturated for negative pressure heads,  $H_p < 0$ . The van Genuchten equations express four properties:

$$Se = \begin{cases} \frac{1}{(1+|\alpha H_p|^n)^m} & H_p < 0 \\ 1 & H_p \geq 0 \end{cases} \quad (2.11)$$

$$\theta = \begin{cases} \theta_r + Se(\theta_s - \theta_r) & H_p < 0 \\ \theta_s & H_p \geq 0 \end{cases} \quad (2.12)$$

$$C_m = \begin{cases} \frac{\alpha m}{1-m}(\theta_s - \theta_r)Se^{\frac{1}{m}}(1 - Se^{\frac{1}{m}})^m & H_p < 0 \\ 0 & H_p \geq 0 \end{cases} \quad (2.13)$$

$$k_r = \begin{cases} Se^l[1 - (1 - Se^{\frac{1}{m}})]^2 & H_p < 0 \\ 0 & H_p \geq 0 \end{cases} \quad (2.14)$$

**Soil saturation**  $Se$  is the soil water saturation and ranges from 0 to 1, representing unsaturated and saturated respectively;  $H_p$  is the pressure head;  $\alpha$  and  $n$  are two van Genuchten parameters, with  $m = 1 - \frac{1}{n}$ .

**Soil moisture content**  $\theta$  is the volumetric soil moisture content or water-filled porosity;  $\theta_s$  is the saturated porosity, i.e. the total porosity of the soil matrix;  $\theta_r$  is



the residual moisture content (even dry soils typically retain some moisture). The soil vapor or vapor-filled porosity is easily calculated by  $\theta_g = \theta_s - \theta$ .

**Specific moisture capacity**  $C_m$  is the specific moisture capacity which dictates the change in  $\theta$  with respect to changes in pressure  $p$ , i.e.  $\frac{\partial \theta}{\partial p}$ .

**Relative permeability**  $k_r$  is the relative permeability and just like  $Se$  ranges from 0 to, representing the soil matrix being fully impermeable and permeable to a particular fluid. The formulation in (2.14) is for water, but the vapor relative permeability is simple  $1 - k_r$ .

In Figure 2.4 the soil water retention curves for sandy loam soils are shown. Notice how the saturation is significantly higher slightly above the groundwater, this is called the capillary fringe and presents a significantly barrier to vapor transport, as we will see in future sections

Figure 2.4: Retention curves for sandy loam soil.

### Richard's Equation

The change in soil moisture through a soil domain is the sum of any change in flux of water in or out of the soil domain. In 1931 Lorenzo Richards[?] developed an eponymous PDE that describes this. Richards' equation itself is an extension of Darcy's Law, which governs fluid flow in saturated media (more on this in section 2.4.2).

$$\rho \left( \frac{C_m}{\rho g} + SeS \right) \frac{\partial p}{\partial t} + \nabla \cdot \rho \left( - \frac{\kappa_s}{\mu} k_r (\nabla p + \rho g \nabla D) \right) = Q_m \quad (2.15)$$

Here  $p$  is the capillary potential;  $C_m$  is the specific moisture capacity;  $Se$  is the effective saturation;  $S$  is the storage coefficient;  $\kappa_s$  is the saturated permeability of the porous media;  $\mu$  is the fluid viscosity;  $k_r$  is the effective permeability;  $\rho$  is the fluid density;  $g$  is the acceleration of gravity;  $D$  is the elevation or head; and  $Q_m$  is a source term, a positive or negative value represent a source or sink respectively.

In the VI model that we are developing we usually assume that there is no change in soil moisture content w.r.t. time, i.e. that it is at steady-state, and that there is no source or sink present, greatly simplifying (2.15). Since we're solving the PDE at steady-state, it is not that important to specify any initial values (although it can reduce computation time), but we need to specify a few boundary conditions to solve (2.15).

### Boundary conditions

In the simplest case only three boundary conditions need to be specified. The first two are Dirichlet boundary conditions<sup>1</sup> where we specify the pressure to be zero at the water table boundary (bottom of the model) and at the ground surface the pressure head is equal the negative of the depth to the water table. The third is a

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<sup>1</sup>A prescribed fixed value to the dependent value at the boundary.

no-flow boundary condition<sup>2</sup>, specifying that there is no soil moisture flux through these boundaries, is applied to all other boundaries.

$$\text{Water table} \quad p = 0 \text{ (Pa)} \quad (2.16)$$

$$\text{Ground surface} \quad p = -z\rho g \text{ (Pa)} \quad (2.17)$$

$$\text{Remaining} \quad -\vec{n} \cdot \rho_{\text{water}}\vec{u} = 0 \quad (2.18)$$

Where  $\rho$  is the density of water;  $z$  is the depth of the water table relative to the ground surface;  $g$  is the acceleration of gravity;  $\vec{n}$  is the a boundary's normal vector;  $\vec{u}$  is the velocity vector of the water moving in the soil matrix.

## 2.4.2 Vapor Transport in Unsaturated Porous Media

Fluid transport in porous media is governed by *Darcy's Law* and was originally formulated by Henry Darcy based on his work on describing water flow through soil under the influence of gravity. Since then it been found to derivable in several ways from the Navier-Stokes equations[?] and may be stated as a pressure gradient driven velocity.

$$\vec{u} = -\frac{\kappa}{\mu}\nabla p \quad (2.19)$$

Here  $\vec{u}$  is the fluid velocity;  $\kappa$  the soil permeability;  $\mu$  is the fluid viscosity; and  $\nabla p$  is the pressure gradient. In VI modeling we're interested in the flow of contaminant vapors but since the contaminant concentrations are typically very low, the transport properties may be taken from those of pure air.

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.

Typically the vapor flows in most VI scenarios are sufficiently slow for the first condition to be fulfilled. And if they are not, there are modifications to Darcy's Law that Most of the contaminant vapor transport takes place in the partially saturated vadose zone and thus, (2.19) 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, we use the relative permeability property,  $k_r$ , from section 2.4.1 is used.

$$\kappa_{\text{eff}} = (1 - k_r)\kappa_s \quad (2.20)$$

Note that in this Darcy's formulation  $(1 - k_r)$  is used to refer to the relative permeability of vapor, e.g. that 0 indicates the soil is completely impermeable for vapor flow (and vice versa).

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

$$\vec{u} = -\frac{(1 - k_r)\kappa_s}{\mu}\nabla p \quad (2.21)$$

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<sup>2</sup>A Neumann boundary condition.

However, (2.21) only gives the vapor velocity as a function of the pressure gradient, to properly model the vapor flow in the soil matrix we need to incorporate Darcy's Law into a continuity equation giving

$$\frac{\partial}{\partial t}(\rho\epsilon) + \nabla \cdot \rho \left( -\frac{(1-k_r)\kappa_s}{\mu} \nabla p \right) = Q_m \quad (2.22)$$

which is governing equation for vapor flow in porous media.

### Boundary conditions

In order to solve (2.22) we need to define some boundary conditions. In our CSM, air is pulled from the atmosphere through the ground surface and into the building via the foundation crack. To model this only three boundary conditions are required.

The first is to define a pressure gauge, i.e. a reference point for where the pressure is zero, which is where air will be pulled from. This is applied to the ground surface boundary. The second is that we apply the indoor/outdoor pressure difference (5 Pa) to the foundation crack boundary. The third type is applied to all remaining boundaries and is a no flow boundary condition, indicating that no flow passes through these boundaries. We also make sure that we specify the symmetry planes present.

$$\text{Ground surface} \quad p = 0 \text{ (Pa)} \quad (2.23)$$

$$\text{Foundation crack} \quad p = p_{\text{in/out}} = -5 \text{ (Pa)} \quad (2.24)$$

$$\text{Remaining} \quad -\vec{n} \cdot \rho \vec{u} = 0 \quad (2.25)$$

where  $\vec{n}$  is the boundary normal vector.

### 2.4.3 Mass Transport in Unsaturated Porous Media

Mass transport of a chemical species occurs primarily through diffusive and advective transport and is typically governed by the advection-diffusion equation (sometimes -reaction is added)

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D \nabla c_i) + \vec{u} \cdot \nabla c_i = R_i \quad (2.26)$$

where  $c_i$  is the concentration of the chemical species;  $t$  is time;  $D$  is the diffusion coefficient;  $\vec{u}$  is the bulk fluid velocity vector; and  $R_i$  is a reaction term. As such the first term is the change of concentration in some control volume, the second and third terms are the diffusive and advective fluxes leaving or entering the control volume, and the fourth is whatever change in concentration due to chemical reactions.

However, this governing equation is too simplistic to accurately model vapor contaminant transport in the vadose zone. As has been discussed before, the transport properties vary significantly in unsaturated porous depending on the soil matrix water saturation. The vadose zone is also a three-phase system, where at any given time some contaminant will be partitioned between the soil, vapor, and liquid phases. The contaminant will also move between these three phases through volatilization/solvation and sorption. To accurately model the mass transport of contaminants through the vadose zone, all of these phenomena must be accounted for.

To rectify this the first term in (2.26) is split to reflect the three phases present.

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial t} \left( \theta c_i + \rho_b c_{p,i} + \theta_g c_{g,i} \right) \quad (2.27)$$

here  $\theta$  is the water filled porosity and its product with  $c_i$  represent the portion of  $c_i$  in the liquid phase;  $\rho_b$  is the bulk density of the soil and  $c_{p,i}$  is  $c_i$  sorbed onto/into the solid phase;  $\theta_g$  is the vapor filled porosity and  $c_{g,i}$  is the volatilized  $c_i$ .

From Richards' equation we get both  $\theta$  and  $\theta_g = \epsilon - \theta$  ( $\epsilon$  is the total porosity of the soil). The bulk density is given by  $\rho_b = (1 - \epsilon)\rho$  where  $\rho$  is the soil density. The sorbed concentration is  $c_{p,i} = K_p c_i$  where  $K_p$  is the sorption isotherm in  $\text{m}^3/\text{kg}$  thus  $c_{p,i}$  is given in  $\text{mol}/\text{kg}$ . The vapor or gas phase concentration is assumed to be governed by Henry's Law and as such  $c_{g,i} = K_{H,i} c_i$  - note that we use the dimensionless Henry's Law constant.

By taking the derivatives in (2.27) and by introducing an effective diffusion coefficient  $D_{\text{eff}}$  in lieu of  $D$  we arrive at

$$\begin{aligned} \frac{\partial c_i}{\partial t} (\theta + \rho_b K_{p,i} + \theta_g K_{H,i}) + \frac{\partial \theta}{\partial t} c_i (1 - K_{H,i}) + \frac{\partial \epsilon}{\partial t} c_i (K_{H,i} - \rho K_{p,i}) \\ + \vec{u} \cdot \nabla c_i = \nabla \cdot (D_{\text{eff},i} \nabla c_i) + R_i \end{aligned} \quad (2.28)$$

here one could add reactions to  $R_i$  to for instance model biodegradation of contaminants. However, since we are interested in modeling VI of TCE, we can omit this since it does not readily degrade.

**Effective diffusivity** The last unexplained part of (2.28) is what the effective diffusion coefficient  $D_{\text{eff},i}$  is. Liquid and gas diffusion coefficients usually differ by orders of magnitude and it is necessary to introduce an effective diffusion coefficient to describe diffusion in unsaturated porous media. This is commonly done via the Millinton-Quirk equation[?]

$$D_{\text{eff}} = D_{\text{water}} \frac{\theta^{\frac{10}{3}}}{\epsilon^2} + \frac{D_{\text{air}}}{K_H} \frac{\theta_g^{\frac{10}{3}}}{\epsilon^2} \quad (2.29)$$

where  $D_{\text{water}}$  is the liquid diffusion coefficient;  $D_{\text{air}}$  is the gas or vapor diffusion coefficient; and  $K_H$  is the dimensionless Henry's Law constant.

## Boundary conditions

As always, some BC are necessary to be specified to solve the PDE governing the mass transport. To model the basic CSM, four different kinds of BCs are required, one for the contaminant source, a second for the sink, third for the entry rate (coupling) with the indoor environment, and fourth are the no flow BCs that have been applied in previous scenarios.

**Groundwater source** In our CSM contaminant vapors emanate from a homogeneously contaminated groundwater source; contaminated with some  $c_{gw}$  concentration. These contaminant vapors can be assumed to emanate from the groundwater according to Henry's Law and the product. The product of the liquid contaminant concentration and the dimensionless Henry's Law constant thus give the vapor contaminant at the interface between the vadose zone and water table.

**Contaminant sink** Any contaminant vapor that reaches the atmosphere is assumed to immediately become infinitely diluted, i.e. that the vapor contaminant here is zero. This is simplest modeled by setting the vapor contaminant concentration to zero at the ground surface boundary.

### Foundation crack entry

**Summary** The last BC is, as in the other cases, a no flow boundary and applied to the remaining boundaries. In summary the following BCs are used.

$$\text{Water table} \quad c = c_{gw}K_H \text{ (mol/m}^3\text{)} \quad (2.30)$$

$$\text{Ground surface} \quad c = 0 \text{ (mol/m}^3\text{)} \quad (2.31)$$

$$\text{Foundation crack} \quad x \quad (2.32)$$

$$\text{Remaining} \quad -\vec{n} \cdot \vec{N} = 0 \text{ (mol/(m}^2 \cdot \text{s))} \quad (2.33)$$

Since the CSM is a steady-state simulation the initial values is not important to specify, but can reduce computation time. If a transient simulation is run the initial values are very important and typically a steady-state solution is used as the initial values.

## 2.5 Meshing

A mesh is a collection of small discrete elements that in combination form a larger geometry or domain. Meshing is the process of generating a mesh. Meshing is perhaps one of the most important and challenging aspects of solving a FEM model and a well-constructed mesh is necessary for accurate and reliable results.

In theory, an infinitely fine mesh will give the analytical solution to a PDE but obviously the computational costs would be infinite then as well; one must always balance the accuracy of the solution and computational resources. This balancing act is somewhat of an art and there are no easily defined rights or wrongs. However, there are general guidelines that are useful to keep in mind while meshing. But before we get into those it is worth to spend some more time on what a mesh is.

The most fundamental unit of the mesh is the element(s) that comprise the mesh. There are many different types of elements that can be used for meshing and choosing which ones to use depend primarily on the spatial dimensionality of the model, the particularities of the geometry, and the physics that we wish to model. Obviously different element types are by necessity needed to model a 2D vs. 3D geometry; you cannot mesh a 3D geometry with 2D squares. This distinction is not very interesting and any lesson learnt about meshing in one of these dimensions is easily generalizable to the other. Thus, we will exclusively discuss the meshing of 3D elements.

There are primarily four types of 3D mesh elements available - the tetrahedral, cuboid, prism, and pyramid - see Figure 2.5. These can be combined in various ways to represent any 3D geometry. The most general out of these is the tetrahedral and will approximate any geometry well. It is not always the most effective choice for meshing a geometry and another element type may be better suited. This is easiest illustrated with an example.

Figure 2.5: Four common mesh elements used to mesh three-dimensional geometries.

Imagine that you are trying to simulate the laminar flow of some fluid through a pipe and been clever enough to realize that by virtue of symmetry only a wedge of the pipe is necessary to be explicitly modeled. We also realize that the flow through the pipe is going to primarily have a gradient in the direction of the flow. In this scenario, it might be beneficial to use prism elements rather than tetrahedrals. Furthermore we could also primarily make the mesh fine in the flow direction while keeping it relatively coarse in other directions. This would allow us to achieve a solution of high accuracy while still keeping the number of elements relatively small.

This is of course a relatively simple example of how an alternative mesh element may be used. For complicated geometries may use all kinds of element shapes in various parts of its domain. These type of multi-element meshes can give significant computational saving but at the expense of often requiring significant user input to be generated. Sticking to one type of elements is often simpler as these can quickly and easily mesh geometries.

Once we have chosen which element(s) to use to mesh our geometry we can move on to creating the mesh. This is done by passing on a series of instructions to a meshing algorithm. Here the user could, for instance, specify the maximum and minimum element sizes, max element growth rate, how finely small features or curves (typically quite difficult to mesh) should be meshed. These instructions can be specific to various parts of the model, e.g. much finer meshing resolution can be specified for an area of interest and vice versa. There are also a variety of specialty mesh features such as a mesh boundary layer available: adding finely spaced mesh layers along a boundary. How to use all of these tools effectively to mesh a geometry is why meshing can be one of the most challenging aspects of FEM modeling.

### 2.5.1 Mesh Study

How does one evaluate that a mesh is sufficiently fine? While there are various metrics that can be useful to determine the quality of a mesh, the most important one is to perform a mesh study. The purpose of a mesh study is to determine the convergence of some property as you increase the fineness of the mesh.

To perform a mesh study you must first define an appropriate metric for the particular problem you want to solve. In vapor intrusion a good choice for this might be the indoor air contaminant concentration, as predicting human exposure is the ultimate goal of VI modeling. The next step is to determine which degree of accuracy is desired (convergence criteria). Create a mesh with the fewest, reasonable number of mesh elements, solve the model, and analyze the results. Iteratively:

1. Remesh the model with a finer mesh.
2. Solve and analyze the results.
3. Plot the result vs. mesh number/ID.
4. Repeat until convergence is met.

In step three we plot the result vs.  $i$ :th mesh, which is the simplest approach, but one could here instead use a variety of mesh metrics instead. The benefit of this would be that you could see which improvement of which specific aspect of the mesh results in a better result, which may make meshing easier. But it can be difficult and usually it is sufficient to simply use your experience and expertise as a guide to determine that your mesh is improved where appropriate.

Figure 2.6: Example result of a mesh study.

## 2.5.2 Meshing The VI Model

Now that we know a little about meshing in general, we can move on and mesh our VI model geometry. The first choice we need to make is which type of element to use, and in order to do that we need to think about the gradients of the dependent variables.

In Richards' equation, the relevant gradient is the capillary pressure gradient, which will go from the water table to the surface, i.e. relatively straight. The Darcy's Law pressure gradient will however not be so straight as we expect a vapor flow from the surface to the building through the foundation crack, forming some sort of arcing streamline; the pressure gradient will be aligned to this streamline. The concentration gradient in the mass transport will likewise have an irregular direction.

Since many of these gradients intersect and go in different directions from each other it makes sense to use tetrahedral elements to mesh the geometry. The aspect ratio between the nodes of each tetrahedra are relatively similar which allows gradients from different directions to be better resolved. Tetrahedral elements are also convenient to use for their simplicity.

Properly meshing our geometry can be a challenge due to the great range of geometric scale. The house and soil domains are on the order of meters while the foundation crack, which is the most important part of the model, is only a centimeter wide. Care must be taken to make sure that foundation crack is finely meshed with small elements (for accurate results) while using larger for the rest of the geometry (to save computation time), i.e. the mesh element size must vary.

Precisely how this is achieved vary depending on the mesh algorithm that you use. `mesh` However, most should be able to automatically mesh the geometry reasonably well by specifying the maximum and minimum mesh sizes, the maximum element growth rate, how finely

Figure 2.7: Our meshed geometry.

## 2.6 Solver Configuration

## 2.7 References