

FINAL REPORT

Tools for Understanding Transients in Vapor Intrusion

ESTCP Project ER-201502

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ACRONYMS AND ABBREVIATIONS

1D	One Dimensional
2D	Two Dimensional
3D	Three Dimensional
AFB	Air Force Base
ASU	Arizona State University
BDF	Backward Differentiation Formula
bgs	below ground surface
CAD	Computer Assisted Design
CPM	Controlled Pressure Method
CST	Continuously Stirred Tank
DNAPL	Dense Non-Aqueous Phase Liquid
ECD	Electron Capture Detector
EPA	Environmental Protection Agency
FDM	Finite Difference Method
FEM	Finite Element Method
FVM	Finite Volume Method
GC	Gas Chromatography
GMRES	Generalized Minimum Residual Method
HVAC	Heating, Ventilation and Air Conditioning
IQR	Inter-quartile Range
ITS	Indicators, Tracers and Surrogates
KDE	Kernel Density Estimation
LU decomposition	Lower-Upper decomposition
MLE	Multiple Lines of Evidence
MS	Mass Spectrometer
MUMPS	Multifrontal Massively Parallel Sparse Direct Solver
NAS	Naval Air Station
PCE	Perchloroethylene (i.e., tetrachloroethylene)
PDD	Pulsed Discharge Ionization Detector
PDE	Partial Differential Equation

RK	Runge-Kutta
SSD	Sub-Slab Depressurization
TCE	Trichloroethylene
VI	Vapor Intrusion
VOC	Volatile Organic Compound

Symbols

A	A generic variable describing area (m^2)
A_e	Air exchange rate (hr^{-1})
c	Concentration ($mols/m^3$ or $mass/m^3$)
c_g	Contaminant concentration in the gas phase ($mols/m^3$ or $mass/m^3$)
c_{ck}	Contaminant concentration at the crack ($mols/m^3$ or $mass/m^3$)
c_{gw}	Contaminant concentration in groundwater ($mols/m^3$ or $mass/m^3$)
c_{gwV}	Contaminant vapor conc. at groundwater interface ($mols/m^3$ or $mass/m^3$)
c_{in}	Indoor air contaminant concentration ($mols/m^3$ or $mass/m^3$)
c_s	Contaminant conc. adsorbed in the solid phase ($mols/m^3$ or $mass/m^3$)
c_T	Total contaminant concentration at any point ($mols/m^3$ or $mass/m^3$)
c_w	Contaminant concentration in the water phase ($mols/m^3$ or $mass/m^3$)
D	Diffusion coefficient (m^2/s or m^2/hr)
D^{air}	Diffusion coefficient of contaminant in air (m^2/s or m^2/hr)
D_{eff}	Effective diffusion coefficient of contaminant (m^2/s or m^2/hr)
D_g	Diffusion coefficient of contaminant in a gas (m^2/s or m^2/hr)
D_w	Diffusion coefficient of contaminant in water (m^2/s or m^2/hr)
e	Estimated local error
h	Height above groundwater (m)
j	A flux (mol/m^2-hr)
j_{ck}	Contaminant flux through breach or crack (mol/m^2-hr or $mass/m^2-hr$)
$j_{advection}$ (or j_{adv})	Contaminant flux due to advection alone (same units as j_{ck})
$j_{diffusion}$ (or j_{diff})	Contaminant flux due to diffusion alone (same units as j_{ck})
k	Permeability (m^2)
k_{ads}	Adsorption rate constant (s^{-1})
k_d	Dry soil permeability (m^2)
k_{des}	Desorption rate constant (s^{-1})
k_r	Relative permeability (dimensionless)
K_H	Henry's Law constant (dimensionless)

K_p	Gas phase contaminant partition coefficient (m^3/kg)
L or L_{slab}	Thickness of a foundation slab (m)
m	A parameter in eq. 2.14 and 2.18
n	An index variable on summations, or a parameter in eq. 2.14
n_{ck}	Contaminant entry rate (mols/time or mass/time)
p	Pressure (Pa)
$p_{in/out}$	Pressure difference indoor-outdoor (Pa)
Pe	Peclet number (see eq. 2.37 or 3.1)
r_{sorb}	Contaminant sorption rate ($mol/m^3 \cdot s$)
R	Reaction rate ($mol/m^3 \cdot hr$)
S_e	Degree of soil saturation by water (dimensionless)
t	Time (usually in hours)
T_g	Gas phase tortuosity
T_w	Water phase tortuosity
u	A general solution to a particular PDE
u_{ck}	Velocity of airflow through a crack (m/s or m/hr)
u_g	Darcy superficial gas flow velocity (m/s)
u_h, u_i	A nodal coefficient (see equation 2.4)
u_w	Darcy superficial water flow velocity (m/s)
v	Velocity (m/hr)
$\mathbf{v}$	Velocity field vector (m/hr)
V	Volume of the impacted building (m^3)
x	Positional coordinate in the plane of the ground surface
x_0, x_n	End node values (see equation 2.4)
y	Positional coordinate in the plane of the ground surface
z	Height, generally above groundwater (m)
α	Parameter in equation (2.14)
α or α_{GW}	Attenuation factor contaminant at groundwater source to indoor air
$\alpha_{subslab}$	Attenuation factor for contaminant from subslab to indoor air
μ	viscosity (Pa-s)
θ_g	Soil porous fraction filled with gas (dimensionless)
θ_r	Soil porous fraction filled with residual water (dimensionless)
θ_t	Total volume fraction of porosity in soil (dimensionless)

θ_w	Soil porous fraction filled with water (dimensionless)
ρ	Density of soil (kg/m ³)
ρ_b	Bulk density of soil (kg/m ³)
ψ_1	A basis function (see equation 2.5)

ABSTRACT

INTRODUCTION AND OBJECTIVES

This study was motivated by recent reports from a number of vapor intrusion (VI)-impacted sites that the measured indoor concentrations of chemicals of concern could vary by orders of magnitude. The sites in question included two that were impacted by operations at military bases (Hill Air Force Base in Layton, UT and Naval Air Station North Island near San Diego, CA) and one studied by the US Environmental Protection Agency in Indianapolis, IN, where the impacts came from nearby former commercial establishments. The objective of this study was to apply numerical modeling to develop an improved understanding of the VI processes at these sites. The goal was also to demonstrate that such modeling tools offer insights that are difficult to develop without such formal analysis, establishing the value of mathematical modeling as a “line of evidence” in analyzing VI scenarios. A further objective of this work was to demonstrate that the tools needed for such numerical analysis are now at a level of development that no particular expertise in numerical analysis is required in order to make effective use of the tools.

TECHNOLOGY DESCRIPTION

The present work has emphasized that use of “ordinary” commercially available finite element solver packages, implemented on desktop computers, can provide powerful insights into the complicated processes involved in VI. The choice was made to use a user-friendly and widely available platform, COMSOL. The goal was to show in a step-by-step way how these tools can be brought to bear in addressing vapor intrusion problems.

PERFORMANCE AND COST ASSESSMENT

The model has been successfully implemented on several different computing platforms. Both the hardware and software costs are modest (a few thousand dollars), requiring only ordinary desktop machines with a bit of enhanced memory and finite element software.

IMPLEMENTATION ISSUES

This report describes earlier VI modeling efforts and then describes how a finite element-based numerical model can be set up. The model is used to discuss what has been learned about the transient processes in VI at the sites that motivated this work. Key conclusions are 1. Orders of magnitude variations in indoor air contaminant concentrations are only possible when there is a confluence of particular site conditions, but variations of one order of magnitude are to be expected given natural variations in air exchange rates and indoor depressurization. 2. The contaminant “entry pathway” determines whether there is significant sensitivity to indoor air pressure changes; when the resistance to sub-slab airflow is significant, the variation of indoor air pressure has a small effect on VI.

KEY PUBLICATIONS

Strom, J., Guo, Y., Yao, Y., Suuberg, E.M. “Factors affecting temporal variations in vapor intrusion-induced indoor air contaminant concentrations” *Building and Environment*, 161, 106196, DOI: 10.1016/j.buildenv.2019.106196 (2019).

Yao, Y., Zuo, J., Luo, J., Chen. Q., Ström, J., Suuberg, E.M. “An examination of the building pressure cycling technique as a tool in vapor intrusion investigations, with analytical solutions” *Journal of Hazardous Materials*, 389, 121915, DOI: 10.1016/j.hazmat.2019.121915 (2020).

A third publication dealing with the modeling of the influence of indoor adsorption phenomena on transients in VI is in preparation.

EXECUTIVE SUMMARY

INTRODUCTION

This study was motivated by recent reports from a number of vapor intrusion (VI)-impacted sites that the measured indoor concentrations of chemicals of concern could vary by orders of magnitude. The sites in question included two that were impacted by operations at military bases (Hill Air Force Base in Layton, UT and Naval Air Station North Island near San Diego, CA) and one that was owned and studied by the US Environmental Protection Agency in Indianapolis, IN, where the impacts came from nearby former commercial establishments. The Hill AFB site will hereafter be referred to as the Arizona State University (ASU) site, because it was owned and studied by that institution. All three sites were heavily impacted by chlorinated solvents, either trichloroethylene (TCE) or perchloroethylene (PCE), and in one case both, which meant that the role of biodegradation in mitigating vapor intrusion were minimal. All three sites were extensively studied and provided a wealth of temporal data not only on indoor concentrations, but also on relevant environmental factors (weather, indoor air exchange, indoor pressure, soil gas concentrations, groundwater concentrations, etc.). Despite the extensive amount of information available on these sites, there remained many aspects of the vapor intrusion processes on these sites that remain unexplained or only partially understood.

In recent years, numerical modeling of vapor intrusion has received increased attention. The development of numerical models of the VI process began with the description of the process offered by Johnson and Ettinger in 1991 (which itself built upon earlier studies of radon intrusion). Since that time, with the growth of computing power and the increase in availability of packages useful for solving the differential equations needed for describing the processes, increasingly detailed models of the VI process have become possible. Such modeling tools offer insights that are difficult to develop without such tools. As a result, mathematical modeling has become established as a “line of evidence” in analyzing VI scenarios. There, however, remains a well-founded skepticism around reliance on modeling alone to provide an understanding of any particular VI situation, since no true “validation” of a model against detailed VI site data has taken place. Even if such a validation were to be made at one site, there would be no basis for a claim that it applies to all sites.

The point made in this work is that reliance on purely empirical methods will generally also be inadequate for developing a complete understanding of VI, without the help of the formal analysis made possible by numerical modeling. The present work has emphasized that use of “ordinary” commercially available finite element solver packages, implemented on desktop computers, can already provide very powerful insights into the inherently complicated processes involved in VI, and help explain the alarmingly large variations in indoor air contaminant concentrations measured at the sites mentioned above.

OBJECTIVES OF THIS STUDY

This project had two distinct objectives. The first was to apply a model that this group had previously developed for describing steady state vapor intrusion phenomena to the transient processes that were of interest and concern at the sites mentioned above. While there had been some limited exploration of transient VI phenomena using the earlier developed models, no results that had been obtained before could begin to explain three order of magnitude variations such as

were reported for the ASU site. Both the ASU site and the EPA site had reported the possibility of preferential pathways, and the previously developed models had not incorporated such pathways in any scenario in which they had a significant effect on the results. Meanwhile, the NAS North Island site did not have a known preferential pathway, and this made clear that the explanation of large variations in contaminant concentrations could not simply be attributed to the existence of such pathways. Hence, there was the need to develop a more robust transient VI model, to include preferential pathways and to use the model to identify which variables would most strongly determine large variations in indoor air contaminant concentrations.

The second objective of this study was to make numerical modeling of the VI process more accessible to workers in the field, and at the same time demonstrate the general value of investing in a modeling effort. The intent was to demonstrate that such modeling tools offer insights that are difficult to develop without such formal analysis, something that has hampered what has been a largely empirical evidence-driven field. This would help further establish mathematical modeling as a useful “line of evidence” in analyzing VI scenarios. There is a well-founded skepticism around reliance on modeling alone to provide a full understanding of any particular VI situation, but the formal analysis involved in modeling will help evaluate different conceptual site models and also to guide the field studies. It also needed to be demonstrated that the mathematical tools required for performing very powerful numerical analysis are now at a level of development such that deep expertise in numerical analysis is no longer required in order to make effective use of the tools. While not yet quite at the level of spreadsheet calculational tools, the user-friendly solver packages now available no longer require computer programming. The present work has moreover emphasized that use of relatively inexpensive “ordinary” commercially available finite element solver packages, implemented on similarly inexpensive desktop computers, can already provide very powerful insights into the inherently complicated processes involved in VI.

TECHNOLOGY DEVELOPMENT

The technology that needed to be developed in this project was the combination of equations required to numerically model vapor intrusion in a transient setting, and their implementation on a finite element solver. The required equations have been worked out some time ago. The key working equations can be summarized as follows:

Calculation of Indoor Air Contaminant Concentration

This equation is quite straightforward. The indoor air concentration is calculated by assuming the building of interest is well mixed and purged by continuous inflow and outflow of air via doors, windows and other air handling equipment that communicates with the outdoor air. By knowing the internal volume of the building (or section of the building of interest, V) and the outdoor air inflow/outflow rate expressed as air changes per time (A_e), the indoor air contaminant concentration is calculated from the contaminant entry rate into the building (n). The resulting indoor air contaminant concentration (c_{in}) is then simply $c_{in} = n/(V \cdot A_e)$. The challenge in vapor intrusion modeling is obtaining a good estimate of n , assuming that the value of V and A_e are known beforehand. In practice, even correctly specifying the values of V and A_e can be tricky, but the real challenge is in calculating a good estimate for n which is the actual key vapor intrusion variable. It should be kept in mind that this value may be time-dependent, defining a scenario in which the indoor air contaminant concentration c_{in} will then also be time-dependent.

The Species Advection-Diffusion Equation

The equation that provides the estimate of the contaminant entry rate n into the building is the contaminant species advection-diffusion equation, which describes the movement of the contaminant through the soil. Normally, the modeling of this aspect of the VI process considers only the vadose zone beneath and surrounding the building of interest. Thus, the region of modeling interest is actually the (partially) dry soil between the top of the water table and the ground surface or bottom of the building's foundation (typically referred to as the foundation slab). It is important to recognize that accounting for the full three dimensionality of the soil surrounding the building is crucial in order to account for certain key aspects of the process.

There are two processes that govern the motion of contaminant vapor in the soil of the vadose zone – advection and diffusion. Since the void space between soil particles in the vadose zone is mostly filled with air, the process of diffusional motion is that of contaminant through air. Diffusion is the process that governs most of the movement of contaminant through the vadose zone, and thus, diffusion determines the concentration profile of contaminant in the soil beneath the building of interest. Advection is of potentially critical importance very near the foundation slab, where it can be driven by the depressurization of the building's interior by a process that is related to the “stack effect”.

A common misconception is that advection is the key process determining contaminant entry into a building. Numerical modeling shows that this is only sometimes true- at times n may be determined by diffusion. It is the critical interplay of advection and diffusion that is generally difficult to understand or predict without the benefit of a numerical model of the advection-diffusion process in the vadose zone. One of the key findings of the modeling work done as part of this study is that a preferential pathway in an environment in which advective flow cannot take place has little influence on VI.

Airflow in the Soil

Darcy's Law has been widely utilized to describe the movement of soil air that plays a role in advective transport of contaminant. Thus, this is another key working equation included in the model of contaminant transport in the vadose zone. This equation must be solved in order to provide an input soil gas velocity profile to the advection-diffusion equation above. One of the features of the vapor intrusion process is that contaminant vapor concentrations are normally so low as to allow solving of the equation governing airflow separately from the equation for advection-diffusion of contaminant.

The Impact of Soil Moisture

One feature of the model developed here involves careful accounting for soil moisture profiles. This aspect has often been neglected in earlier modeling work. Soil moisture “blocks” the pore spaces between soil grains in the vadose zone. This reduces both the diffusivity of the contaminant in the soil as well as the permeability of the soil for advective flow. Both processes are important, and thus correct accounting of soil moisture profiles is vital to reliable modeling of the rate of contaminant transport. In this work, the estimates of soil moisture profile recommended by van Genuchten have been adopted along with the accompanying estimates of soil permeability for advection. Meanwhile, the Millington-Quirk expression for estimating contaminant diffusivity in moist soils has also been used.

Implementing the Model in COMSOL

In order to obtain an estimate of the entry rate of contaminant into a building of interest, the above differential equations need to be solved on a domain, an area in space, which includes the building. The choice was made to employ an off-the-shelf finite element solver package that has a straightforward user interface, which is described in this report. The choice of COMSOL was based upon an earlier comparison with other similar packages, and the choice was dictated by a perceived ease of use and reasonable cost. None of the conclusions of this study depend upon use of this particular package. But the choice to standardize on this one package was motivated by a desire to produce a step-by-step description of how to go from the statement of the basic equations through their implementation in a solver to display of results.

There are two steps that need to be taken in order to effect the solution of the VI model defined by the above equations. The first is to formally define the domain, as a three-dimensional grid. The COMSOL package has built in features that permit this to be done fairly easily for a simple geometry. The relevant working equations are already pre-programmed into this particular solver package, so no programming is needed in order to solve these differential equations. All that is required is to define the physical properties in the equations and the boundary and initial conditions for their solution. This report serves as a full manual for taking these steps.

PERFORMANCE ASSESSMENT

The model described above was applied to a physical situation that was intended to mimic key features of the ASU site. Once the available data describing this site had been carefully examined, it was realized that it would only be possible to model the key features of the site rather than preparing an exact replica of the ASU site; there were simply too many details of site geometry that could not be precisely defined. This did not prevent the very successful use of the model to predict actually measured key trends in, and magnitudes of, contaminant concentrations in a transient scenario. Very good agreement obtained between the actual measured indoor contaminant concentrations as a function of indoor pressure.

Once it was demonstrated that the model could reasonably predict the behavior of this site, it was used to examine the sensitivity of its predictions to key variables. The results of this analysis showed that it was actually a unique combination of site features that led to the observed large swings in indoor air contaminant concentration. A preferential pathway (in this case, a land drain) delivering contaminant to the sub-slab zone directly beneath the foundation could not by itself lead to the observed result. What was simultaneously required was a mechanism for delivering air to the permeable gravel sub-base that communicated with the building's interior. Absent either of these factors, the observed large swings in indoor air contaminant concentration could not be generated. This indicated that the scenario at the ASU site would not necessarily be expected at a great number of other sites. This was further confirmed by modeling the situation when the land drain beneath the site was closed, in which case the roughly one order of magnitude variation in indoor air contaminant concentrations could be predicted based solely upon the natural variability in air exchange rate and indoor air pressure fluctuations.

It needs to be emphasized that the model was not being tested against actual absolute values of indoor air concentration at the ASU site. There was no single concentration value that could be used for such a comparison, since concentration varied throughout the building. As also noted before, there were physical aspects of the real site that were not, or could not be, measured with enough accuracy to permit an actual replica of the site to be modeled. The model of the ASU-like site did, however, perform well in terms of predicting actual measured trends in indoor air contaminant concentrations and it was certainly close to actual measured values in its predictions.

The insights obtained from modeling the ASU site raised a question of why then, in the absence of a preferential pathway, the NAS North Island site could also show several order of magnitude swings in indoor air concentration. In this case, the answer became obvious in examining the relative magnitudes of the pressure driving force at NAS North Island vs. the ASU site. North Island showed very large indoor pressure swings. It also had a fairly permeable soil underneath the foundation. In that case, the advectively driven entry of contaminant was responsible for the observed transients.

The modeling also indicated why the “controlled pressure method” of examining vapor intrusion gives different kinds of results at different sites. Controlled pressure testing is used at VI sites in an attempt to create a “worst possible case” result for vapor intrusion in a particular building. In this test, a building is deliberately depressurized in an effort to maximize the entry rate of contaminant and thus maximize indoor air contaminant concentration. Inherent in this method is an assumption that advective entry is an important mechanism for contaminant entry. But as was learned from the sensitivity testing performed in connection with the ASU site modeling, if the sub-slab soil is not itself permeable, or if permeable, not connected to a source of air, then depressurization cannot significantly increase contaminant entry rate because advective entry cannot increase. This analysis was characterized in terms of the Peclet number governing entry of contaminant via foundation breaches in the building. The Peclet number is defined as the ratio of advective entry rate to diffusional entry rate. For a highly impermeable sub-foundation soil, the value of the Peclet number is low, and largely unaffected by small variations in indoor depressurization.

The model in this study has thus shown itself to be of significant value in predicting the factors governing variations in contaminant entry rate. The main project conclusions can then be summarized as follows:

- The large variations in measured indoor air contaminant concentrations at the ASU site had their origins in the existence of a combination of a preferential pathway combined with a ready source of air supporting advective entry of contaminants into the building. Absent either factor, there could not have been nearly as large a variation.
- The large variations in the indoor air contaminant concentrations at NAS North Island did not involve a preferential pathway, but were driven by an unusually high indoor depressurization in the presence of a permeable soil.
- Results from the ASU site suggest that variations of an order of magnitude in indoor air contaminant concentrations should be expected simply on the basis of the combined effects of air exchange rate and indoor depressurization effects.

- The generally assumed dependence of indoor air contaminant concentrations on the extent of indoor depressurization will not always be observed, if the entry rate of contaminant is diffusion controlled, as might be expected at many sites. This may limit the value of controlled pressure measurement characterizations of vapor intrusion potential. This might also be viewed as challenging the assumption that cold-season indoor air sampling will always lead to the most conservative result.

COST ASSESSMENT

The model has been successfully implemented on several different computing platforms. Both the hardware and software costs are modest (a few thousand dollars), requiring only ordinary desktop machines with a bit of enhanced memory and finite element software.

IMPLEMENTATION ISSUES

There is very little that prevents much greater use of numerical modeling tools such as those described and used here to develop a better understanding of vapor intrusion issues. The methods are well developed and the use of modern solver packages enables even new users to quickly obtain results.

The key impediments to greater use of numerical modeling in examination of VI scenarios are

- The traditions in the field are such that it is highly empirical. This is certainly understandable. There is a health risk associated with exposures that involve concentrations so low that they normally cannot be sensed by smell and their measurement requires sensitive instrumentation. Thus a conservative approach to protection of human health demands actual measurements be made in order to assess the scope of the problem. The field is also dominated by the belief that there is no acceptable surrogate for performing actual indoor air sampling. Once indoor air sampling has been determined to be necessary and data of that kind have been gathered, it would be understandable that modeling of the situation could be viewed as almost superfluous.
- Related to the above, there has never been what those in the field would consider a true “validation” of a numerical model of vapor intrusion. Nor is it likely that any one attempt at validation, even if successful, would fully address this concern. The reality is that part of the complexity of vapor intrusion arises from the fact that no two sites are ever alike. This is seen in the neighborhood of the ASU site outside Hill AFB. Different nearby homes have very different situations vis-à-vis the severity of vapor intrusion impacts. And there is the added issue that most modeling has involved fairly small structures, and that capture of the complexity of a large industrial or commercial site might be very difficult.
- There remains a belief that to properly perform numerical modeling of vapor intrusion still requires a significant investment of time in learning the techniques.

These are all valid points. Hopefully, the third point has been somewhat addressed by preparation of this manual, that has attempted to provide a straightforward “roadmap” for those seeking to perform such modeling. Regarding the first point, it has never been envisioned that modeling would entirely replace actual field sampling. Instead, what it is hoped that modeling will provide is an additional line of evidence that can help in understanding the complexity of a site.

If field measurements provide results that cannot be reconciled with a reasonable model of the site, this can indicate that the site conceptual model is somehow flawed (e.g., that the existence of a preferential pathway has been overlooked). In this case, the model can serve as a basis for guiding further investigation of the site. Thus rather than modeling standing on its own and requiring validation in that regard, instead, it serves to help validate the conceptual site model that is developed based upon field measurements. Finally, it is often overlooked that a model that does capture the key aspects of a site can be a useful tool for designing a mitigation response for that site; it allows trying out different types of designs (e.g., for subslab depressurization) before a decision is made as to their implementation.

1.0 INTRODUCTION

1.1 INDOOR AIR QUALITY AND VAPOR INTRUSION

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, radon gas, or other airborne pollutants. Since industrialization the number of potential hazardous pollutants has increased significantly, along with concerns about air quality. At the same time, people spend more time indoors now than ever before, with Americans spending up to 90% of their waking time indoors [1]. This has resulted in increasing attention to issues related to indoor air quality.

Some early scientific inquiries into indoor air quality focused on pollutant sources that were generated in the home, e.g. by heating and cooking systems, and these types of pollutants are still relevant today, but of particular concern in developing countries [2, 3]. Many building materials can also cause indoor air quality issues, with exposure to asbestos fibers being perhaps one of the best-known examples. Mold is another common indoor air quality concern [4].

In the 1970s, in response to growing public health concerns, research began into indoor exposure to radon gas. Radon gas, which is radioactive and which is generated by the decay of naturally occurring uranium in soils and rocks, was discovered to be entering buildings, resulting in chronic exposure of the inhabitants [5]. Exposure to radon gas can significantly increase the risk of developing lung cancer, and is presently the second leading cause of lung cancer (after smoking) in many countries [6]. With the recognition of the hazard posed by radon intrusion into buildings, the same concerns were soon recognized relative to entry of anthropogenic contaminant vapors via the same soil pathway. With that the formal investigation of the vapor intrusion (VI) problem began.

Vapor intrusion involves the migration of contaminant vapors from a contaminant source in the soil into overlying buildings. These contaminants evaporate from a source, which is often contaminated groundwater, percolate through the soil of the vadose zone, and enter a building through breaches or openings in its foundation, e.g., cracks in the foundation slab, gaps between walls and floors, sump pits, or other utility openings [7]. Much early VI research was heavily influenced by the work previously performed by radon intrusion researchers, who studied these same pathways.

Vapor intrusion of volatile organic compounds (VOCs) differs from radon intrusion in some important ways. Many of these differences stem from the properties of the contaminants themselves, beyond the fact that the other VI contaminants of concern are of anthropogenic origin. Radon is unstable due to radioactive decay, and has a half-life of around 3.8 days (for Rn^{222} , the main natural isotope of radon). This is not the case with other contaminants of VI interest [8]. The radon decay occurs during its transport through soil, which has no analog in VI involving VOCs, although some VOCs of VI concern can also be biodegraded by bacteria in soil [7, 9].

As already noted, in VI involving VOCs there is often a contaminated groundwater source underneath the impacted building, and the source of the groundwater contamination typically is traced to a spill or release of the contaminant in the surrounding area. There may be any number of processes that lead to such releases [7]. A release from a single source can impact a large number of buildings. The US Environmental Protection Agency (EPA) notes that among its over 1000 Superfund sites, many contain the contaminants of potential VI concern [7,10].

Many of the contaminants of concern do not readily degrade, and thus legacy contamination from events many years ago is an issue [7]. Contaminated groundwater is only one type of potential VI source, and “free product” in soils can often be the cause of, or contributor to, VI. Figure 1.1 illustrates some common aspects of VI pathways.

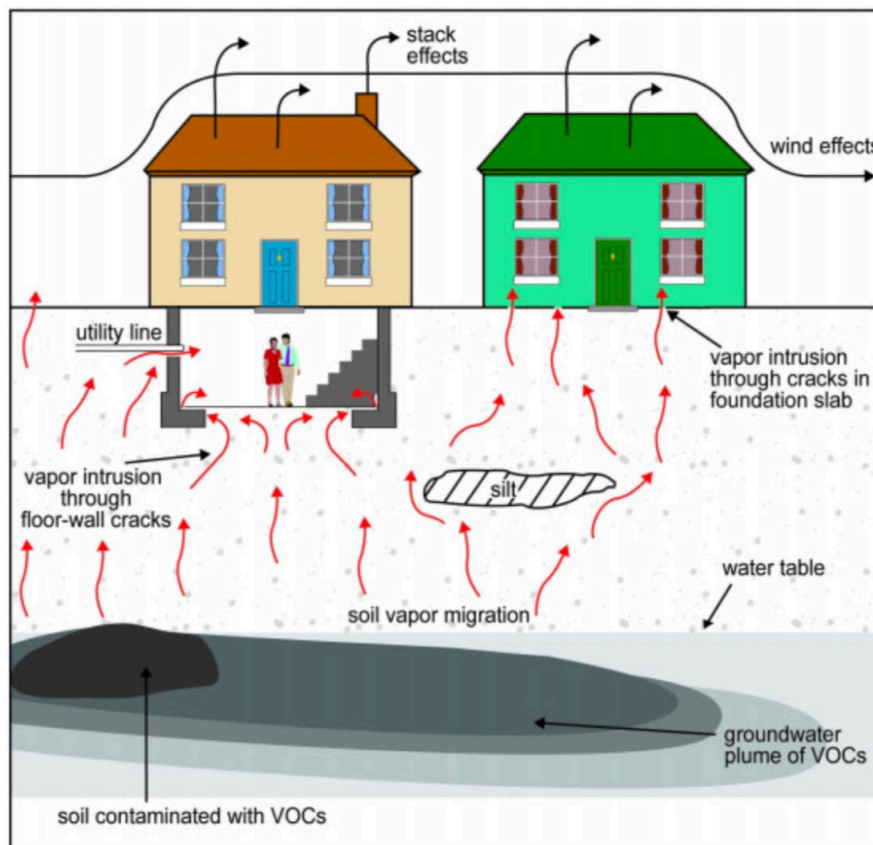


Figure 1.1. Vapor Intrusion into a Building Can Occur by a Variety of Different Pathways, But Always Involving Some Aspect of Transport Through Soil.

Figure from the EPA [11].

Some common contaminants of VI concern are chlorinated solvents such as trichloroethylene (TCE), tetrachloroethylene (or perchloroethylene, PCE), or chloroform. Various petroleum products such as benzene as well as other volatile organics are also of concern. Of the various VI contaminants, TCE has emerged as being of particular concern. TCE is an excellent degreaser and has been extensively used commercially and by the military [7]. The concern over TCE is partly due to its associated cancer risk and partly because it was recently hypothesized to possibly play a role in birth defects [12], though there remains some question about this [13]. Regardless, TCE is carcinogenic and the concentration levels of concern for both long term and short term exposure are very low (at levels of $\mu\text{g}/\text{m}^3$). The fact that there is widespread TCE contamination at concentration levels of concern is what has made this one of the key compounds of VI interest, and it was a main focus of this study as well.

Determining if VI occurs at a particular site is often challenging. Because sensitive measurement equipment is normally needed for its detection, the occupants of impacted buildings normally do not know of the existence of a problem. When VI is investigated, there is often no alternative to performing indoor air measurements, which is both alarming to, and inconvenient for, the building occupants as well as costly and inconvenient for the investigator. Partly because of the reality of limited access to what are often large numbers of impacted structures, VI investigations have not always been as thorough as investigators might have preferred. Thus, while VI has been studied for decades, many questions and challenges remain, in particular with regards to characterizing the great spatial and temporal variability that exist both within and between VI sites [7]. The VI investigation field has been dominated by empiricism, based upon the field data that have been collected. While there has been good progress made using this approach, the power of formal mathematical modeling of VI has really not been realized as yet. It is this aspect of VI investigation that this report addresses.

1.2 ISSUES IN VAPOR INTRUSION INVESTIGATIONS

Determining if vapor intrusion occurs at a building is often difficult. Simple indoor air collection and analysis is too simplistic and can easily yield false positives. Many common consumer products contain the same contaminants that are of concern in VI, and the presence of these products in the home may be an important source of the compounds of concern in the indoor air environment. Many contaminants may be inadvertently introduced, such as by bringing home newly dry-cleaned clothing (a common source of PCE). During formal VI investigations, great care is taken to eliminate such indoor sources but this can be challenging [7]. What has been less recognized is that the contaminants of concern can also sorb onto/into various household materials and subsequently desorb for significant periods of time, potentially temporally extending the influence of sources beyond the time of their removal [14, 15]. This will be explored in this report as part of the analysis of causes of transients.

Often, the first indication of a potential VI issue comes from a finding of contamination in groundwater. However, even identifying such a potential source is not enough evidence of VI, as the presence of a contaminant source does not mean that the contaminant vapor actually enters the overlying building. Folkes et al.[16] conducted a decade long study of VI sites in Redfield, Colorado, and a 19 month long study in New York, which showed that many of the sites, even though they were above a contaminated groundwater source, were not impacted by VI. Taking a different approach, some VI investigators believe that sampling of the soil gas beneath the foundation of a potentially impacted building can confirm a VI pathway. The presumption is that such sampling can reveal a concentration gradient in the “correct” direction from soil gas to indoor air. However, as work by Holton et al. [17] has shown, contaminant vapors in the indoor environment may actually migrate from inside the building to the subslab, creating a contaminant “cloud” in soil beneath the building that may persist for significant periods of time.

Despite the above complication, sampling of soil gas from the source to the indoor can often establish what is termed a “completed pathway”. The decrease in contaminant vapor concentration from source to indoor air is called “attenuation” and is quantitatively given by the ratio of concentration at a “downstream” sampling point to that from an “upstream” point (closer to the source).

This ratio is termed the attenuation factor. One widely used form of the attenuation factor is the indoor air contaminant concentration divided by the contaminant vapor concentration at the soil-gas ground-water interface. The symbol α is used in this work (as in most of the VI literature) to denote attenuation factor and a subscript will denote which measurement points are being considered. In the case of characterizing attenuation relative to a groundwater source, the contaminant vapor concentration at the groundwater interface is generally assumed to be given by Henry's Law ($c_{\text{gwV}} = K_{\text{HC}} c_{\text{gw}}$), where c_{gwV} is the vapor phase concentration at the groundwater interface and c_{gw} is the water phase concentration of contaminant. This simple picture of a well-defined vapor concentration at the groundwater interface has been widely used, but is problematic as will be discussed further below.

Over time, the EPA has compiled data on attenuation factors relative to both groundwater source and the soil gas immediately below a building foundation (the so-called subslab). Using these data, recommendations regarding "typically expected" attenuation factors have been established to help guide investigators and regulators in determining the VI risk. But the empirically based values are subject to orders of magnitude uncertainty. For instance, the EPA recommends that an attenuation from the subslab region to the indoor of $\alpha_{\text{subslab}} \approx 0.03$. In reality, attenuation factor values can vary by orders of magnitude due to the influence of many variables, and such recommended values can therefore be too conservative [18]. Some of the factors influencing attenuation factors are soil heterogeneity, non-homogeneous contaminant source concentrations, as well as differences in the nature of the source (e.g. groundwater vs. free product). These can all also contribute to significant spatial variability in contaminant concentration at a site. A good example of this is seen in a study by Luo et al. [19] where contaminant vapor concentration beneath a building foundation varied from 200 to less than 0.01 mg/L. Bekele et al. [20] also found at another site that TCE soil gas sub-foundation concentrations could vary by an order of magnitude.

Not all indoor air environments are perfectly mixed and indoor contaminant concentration can vary significantly between different rooms or compartments in a building for reasons that might not always be apparent. This was the case for a site reported on by Pennell et al. [21] who found that the indoor contaminant concentration was significantly higher in an upstairs bathroom than in the building's basement, where higher concentrations are typically expected. In that case, the "strange result" had to do with the existence of a preferential sewer pathway into the upstairs bathroom. A preferential pathway is a term used to describe a conduit or some naturally occurring pathway through the soil that permits enhanced contaminant vapor transport from a source to very near, or into, a building. This is in contrast with the more "traditional" view that contaminant transport occurs by diffusion through the soil.

Preferential pathways play a key role in determining the behavior that is the main subject of this study. The concept of a preferential pathway was illustrated in Figure 1.1 as a utility line that enters a house; such a line can carry contaminant vapors directly into the structure, bypassing the soil transport route. McHugh et al. [22] studied the EPA VI study site in Indianapolis, and concluded that the sewer system there acted as a preferential pathway bringing contaminants into the house (in addition to the soil pathway from the contaminated groundwater). This site exhibited significant temporal variability in indoor air concentrations [8]. Guo et al. [23] studied the VI impacted house near Hill AFB in Layton, UT, and it was also found to be impacted by a preferential pathway- in that case, a land drain that allowed contaminant vapors to be transported from a sewer to the near-slab region beneath a house (and close to a visible breach in the foundation).

Holton et al. [24] demonstrated the very significant temporal variability in indoor contaminant concentrations that can be caused by such a pathway, as they found close to four orders of magnitude temporal variability in measured indoor air contaminant concentrations during the multi-year study period at this site. The preferential pathways at both sites are a significant focus of the modeling work performed here.

Not all significant contaminant concentration temporal variations are, however, associated with preferential pathways. Hosangadi et al. [25] studied the Naval Air Station North Island VI site in San Diego, CA, that likewise showed orders of magnitude temporal variability in measured indoor air contaminant concentrations. There was no obvious preferential pathway involved in that case. Again, we believe that the modeling work to be presented below can explain that observation, and how that situation differed from those that existed at the Hill AFB and EPA sites.

The temporal variability in indoor air contaminant concentrations typically exhibits seasonality, and highest indoor contaminant concentrations are often found during the colder months of the year [8, 24], although there are cases where the opposite is true. For example, Steck et al. [26] showed this at a radon impacted building in Minnesota, where the highest radon levels were observed during summer. Some authors such as Bekele, et al. [20] suggest that it may be necessary to collect samples at intervals across a full year, to account for all seasonal effects.

Thus, the complexity and nuances of VI have made it necessary for a multiple lines-of-evidence (MLE) approach to be adopted when determining if a building is impacted by VI [7, 27]. However, numerical modeling, while recognized as one of the possible lines of evidence, has not yet been fully enough utilized in exploring the complexity of many sites.

1.3 NEW TECHNIQUES IN FIELD INVESTIGATION OF VAPOR INTRUSION AND HOW NUMERICAL MODELING CAN ASSIST IN INTERPRETING THE RESULTS

A number of new in-the-field investigatory techniques and methods have been proposed, but in general their efficacy is yet to be fully established [28]. This is because they have not yet yielded consistent results. We believe that the modeling techniques developed here can offer new insights into when and how these new investigation techniques can be usefully applied.

The Controlled Pressure Method

Many buildings are naturally at a slight (few Pa) depressurization or over-pressurization relative to atmosphere due to the operation of heating, ventilation, and air conditioning (HVAC) systems. In non-commercial buildings, this typically gives rise to an interior depressurization as a result of the “stack effect”, as displayed in Figure 1.1. This depressurization can induce a flow of (contaminant-containing) air from soil into the building. Building upon this conceptual model, the controlled pressure method (CPM) has been developed, in which blowers or fans are used to control the extent of depressurization (or over-pressurization) of a building (see Figure 1.2). The basic idea has been to create a “worst case” scenario in which contaminant soil vapors are induced to enter the building at a greater than natural rate. In fact, Guo et al. [23] used the technique to examine the influence of a preferential pathway at their study site near Hill AFB. Conversely, over-pressurizing a building can then theoretically prevent contaminant entry from the subslab

zone, potentially allowing identification of the existence of indoor contaminant sources, since the presence of contaminant vapors in the indoor environment of the over-pressurized building could “only” be the result of an indoor source [30]. The difficulty is that there is not yet clear guidance of what pressures are “best” and when indoor air contaminant concentration measurements should actually be made during a testing cycle. This issue has been discussed in a recent publication [31]. Once again, numerical modeling can point in a direction that clarifies these issues, as will be discussed below.

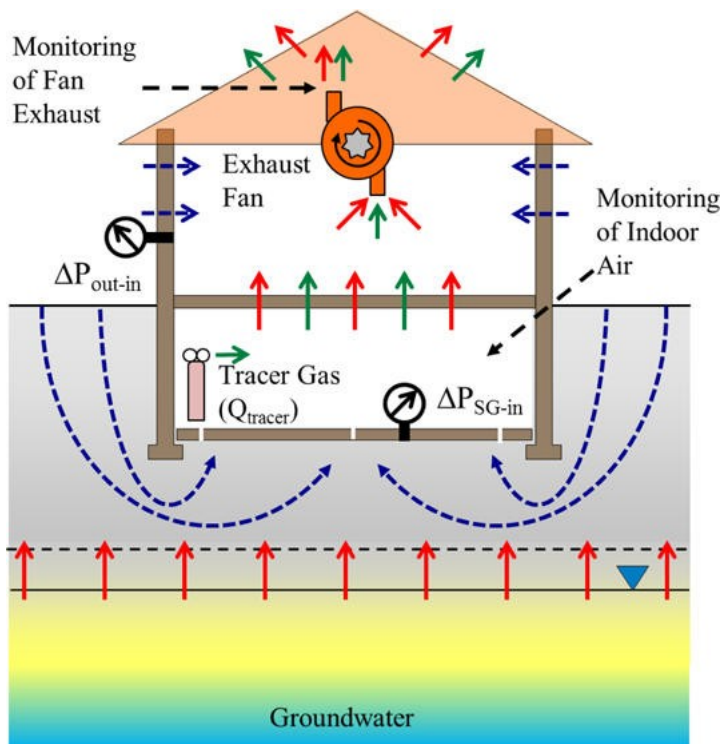


Figure 1.2. Conceptual Scheme of the Controlled Pressure Method.

A VI impacted building is depressurized to a greater than natural extent, using a blower. This theoretically increases the contaminant entry rate into the building. Figure from Holton et al. [29].

Indicators, Tracers, and Surrogates

The spatial and temporal variability of VI raises concerns regarding false positives and negatives. While continuous monitoring of indoor contaminant concentrations or increased sample collection frequency could theoretically address this issue, this approach is not practical, especially when numerous sites with many buildings are involved. Thus, there is a desire to develop guidelines that help reduce the sampling requirements while retaining confidence that the relevant (i.e., highest) levels of VI contamination have actually been determined [32]. To address this need, the use indicators, tracers, and surrogates (ITS) has been suggested as a way of determining when to conduct a VI site investigation. For example, it may be asked under what meteorological conditions is it likely that the 95th percentile indoor contaminant concentration will be found [32]? Once again, use of numerical modeling can help identify which parameters should have the greatest influence on indoor air contaminant concentration variability, giving greater confidence and fundamental basis to this technique.

1.4 MATHEMATICAL MODELING OF VAPOR INTRUSION

Having suggested that mathematical models of VI can help in understanding the processes, it is not surprising that there have already been many efforts in that direction. This section will only briefly review the many mathematical models that have already been used to describe the VI process. A comprehensive review of the models developed up to that point in time was presented in 2013 [33], and will not be repeated in any great depth here. There have been a large number of different VI models presented in the literature, including several that have appeared after the cited review. It is important to note that these many modeling efforts have been different in certain major or subtle ways that can make a significant difference in what they can reliably predict.

Most of the early VI modeling work adapted approaches developed for predicting radon intrusion [e.g., 34-37]. The soil transport portion of these models could be traced to even earlier work on movement of pesticides in soils [e.g.38]. Later work in the radon modeling field established the key role that indoor depressurization could play in determining transport of that contaminant from soil into the structure [39-41]. One of those articles actually concluded a role for a sub-foundation gravel sub-base that is quite similar to that which we have concluded regarding its importance in VI systems. In parallel with the development of the later radon intrusion models Johnson and Ettinger [42] developed what was to become the best known and widely used VI model. This was a one-dimensional transport model describing the vertical transport of VI contaminants from a groundwater source through the vadose zone, into an overlying building. The EPA adopted this model as the basis of a spreadsheet VI screening tool and it has seen widespread use [7]. This model has the shortcoming of being one-dimensional- that is, lateral diffusion of contaminant vapor cannot be accounted for. On the other hand, it is computationally very simple. A formal comparison of its predictions with those of a full three-dimensional numerical model (using the same input parameters) has shown that the predictions of the one-dimensional model are generally reasonable, though in different cases they can either be higher or lower than those of the more complete representation [43].

One of the virtually universal conclusions from the beginning of VI modeling is that transport from the source through the soil of the vadose zone is almost invariably controlled by diffusion; it is only very near the foundation of the impacted structure that the small stack effect-induced pressure differentials can cause a significant advective flow of soil gas. For describing the diffusive transport, an approach to estimating effective diffusivity in soil, recommended by Millington and Quirk [44], is generally adopted. This method will be discussed below.

As facilities for performing computations became more generally accessible, many more advanced models requiring numerical solution were developed. These models allowed for more physical features to be included and for more complicated VI scenarios to be examined. These included the numerical models developed by Abreu and Johnson [45] and Pennell, et al. [46]. The major difference between these models has only been in the solution method; Abreu and Johnson relied on a finite difference technique, whereas Pennell et al. solved the model using a finite element method, described below.

Since the time that the above-cited VI modeling review [33], there have been other developments and improvements to the basic model structure. For example, Shirazi and Pennell have incorporated wind and stack effects into the basic three-dimensional model [47]. Several groups have incorporated biodegradation processes into full three-dimensional fluid flow models, in order to account for these in petroleum vapor intrusion [48-50]. The potential importance of soil moisture fluctuations was pointed out by Tillman and Weaver [51], and this realization led to more careful consideration in three-dimensional VI modeling of processes such as rainfall events [52] and the role of soil moisture profiles generally, including the very important resistance of the capillary zone [53]. In this latter regard, the incorporation of the very important soil moisture profile model of van Genuchten [54] will be featured prominently in the modeling described below. The importance of statistical fluctuations of model input parameters has also been considered using the Johnson and Ettinger model [55], and this will also play an important role in modeling the temporal variability of results, as discussed below.

Soundly constructed mathematical models can serve as a valuable tool in helping develop further understanding of complicated VI phenomena. Such models have already been used to investigate topics such as the role of soil moisture in VI transport [53], how different foundation features affect contaminant entry [56], or how wind and outdoor temperature affect building air exchange [47]. In this report, the focus is on transient phenomena in VI. Some limited modeling studies of transient phenomena have been previously presented [e.g., 57, 58], but these did not fully explain the large temporal variations observed at the main sites of interest in this project.

The next section of this report outlines the basic structure of three-dimensional numerical models of vapor intrusion and how these are implemented in an appropriate solver system. The choice was made early on in this project to rely upon a commercially available, and relatively user-friendly, solver (COMSOL). This choice was made in order to encourage use of the tool by those who might have had only limited exposure to formal numerical modeling of fluid flow systems. There is nothing to prevent implementation of the model in any other solver that permits dealing with the time-dependent partial differential equations that characterize the problem.

2.0 NUMERICAL MODELING OF VAPOR INTRUSION

2.1 SUMMARY

This section presents an example of development and solution of a numerical model that simulates VI. The choice is made to simulate a residential house-scale building, overlying a contaminated groundwater source. This is a typical scenario that has been explored in most three-dimensional numerical modeling studies. There is no reason why the same methodologies cannot be applied to larger structures. The limitation might come in with respect to how large a building can be considered while at the same time preserving the fine scale detail that may be necessary around contaminant entry points into the structure. Even this is not a real limitation of the method so much as of the software-hardware combination that is needed to solve the model. The goal of this project has been to offer models that are implementable on ordinary desktop computers, rather than large mainframes or supercomputers.

As a starting point, the physics and associated governing equations required to model a typical VI scenario are presented, along with the necessary initial and boundary conditions to solve these equations. The solution of the modeled system, using the finite element method (FEM), is then briefly described. Practical considerations in implementing the FEM solution are covered - including geometry and mesh generation, solver configuration, and post-processing of results.

2.2 INTRODUCTION

To illustrate the formulation of a mathematical description of VI, a simple hypothetical VI scenario is considered. Initially, a steady-state situation is examined. This means that all chemical and physical processes have reached steady values- there is no time-varying behavior. While the description of transients is a principal focus of this study, it is generally easier to begin with a steady state analysis of the basic process. The phenomena are complicated enough that examination of a steady state scenario will help inform and guide a subsequent transient analysis, which is more elaborate and requires more computational time.

It is important to emphasize that the main portion of the model to be developed focus exclusively on the transport of contaminant vapor from a source in the ground or groundwater through the vadose zone to the boundary defined by the foundation of a structure of interest. It is the concentration of contaminant vapor at entry points at the foundation boundary that determines its entry rate into the structure. Thus, the model to be developed is fundamentally a vadose zone transport model. The actual entry rate into the structure will be modeled using very simple equations describing transport through breaches in the foundation, either via diffusion or advection or a combination of the two. This entry rate will be combined with a very simple description of the volume in the structure that is impacted and the air exchange rate within that volume, in order to estimate an indoor air concentration. But despite this last step, it is still important to bear in mind that the model to be developed really only describes transport through the vadose zone, and that it is this that enables estimating the entry rate and from that, the indoor air contaminant concentration.

The model will be developed for a house with a 10 m by 10 m foundation footprint. There is no particular reason why a structure with a square footprint must be chosen- it is done here purely for convenience of representation. To the extent that modeled structures do have a form that allows defining planes of symmetry, there can be a savings in terms of the size of the mesh that needs to be defined (see below). This structure is assumed to have a basement whose foundation slab lies 1 m below ground surface (bgs). Again, this choice is arbitrary, and modeling has been applied in many cases to structures with deeper basements or no basement at all (slab-on-grade construction).

The nature of the contaminant vapor entry pathways into the structure requires careful attention. It has been shown in previous three-dimensional numerical modeling using the same model as described here that, except in the case of preferential pathways, it is really the area of breaches (i.e., cracks, holes) in the foundation slab rather than their particular geometry, that is critical to predictions of entry rate [56]. Thus it is important to have some idea of how much communication area there is between soil and indoor air, but the exact location of the cracks or breaches contributing that area is less important. Of course, the more information that is available to describe the cracks or breaches, the better the model can do at predicting details of VI behavior. For the purposes of this sample model, it is assumed that there is a 1 cm wide crack between the foundation wall and the slab, running along the perimeter of the 15 cm thick impermeable foundation slab. It is only through this crack that all contaminant vapor entry into the house is assumed to occur.

The next choice that is required concerns the volume of the structure that is impacted by vapor intrusion. Sometimes this is taken to be the volume of the whole structure. Generally, however, a structure is divided into different levels and rooms, some of which are closer to the vapor entry routes and others more distant. It is rare that an entire structure has air that is perfectly mixed between all rooms. In analysis of vapor intrusion, since the main interest is in the areas of highest risk to human health, the choice is often made to focus on the volume of rooms that are closest to the entry points. In the case of this sample analysis, the basement is chosen as the control volume for which the indoor contaminant concentration will be determined. This basement is arbitrarily assumed to have a ceiling height of 3 m, thus giving a total volume of 300 m³ for that space.

Another key choice is that of the relevant air exchange rate for the control volume of interest. Generally, houses exchange air with the outdoor environment. This is an important feature of house design. Houses that are built too “tight”, perhaps for reasons of energy conservation, run the risk of developing “sick building syndrome”, as vapors, including CO₂, from indoor activities build up. Thus, it is common for all structures to be built with an allowance for exchange of air with the outdoors. Here, the air exchange rate with outdoor air is assumed to be 0.5 h⁻¹, meaning that half the air in the selected control volume is exchanged with outdoor air every hour. In this process of air exchange, the contaminant vapors are expelled along with the rest of the building air, at a concentration characteristic of the whole volume. It is typical to assume that within a control volume, the concentration of contaminant vapor is uniform as the air within the whole control volume is well mixed by normal air currents. It is clear that many different assumptions can be made regarding the indoor air and its mixing; there are many models that describe indoor air mixing, as this is a key consideration in design of HVAC systems. Here, since the focus is mainly on the vadose zone transport portion of the process, these models will not be incorporated, but there is no reason why they cannot be.

The next key choice regards the nature of the contaminant source. As already noted above, it is quite common to assume the vapor source is contaminated groundwater, but there are many instances in which there might be a contribution of free product within the vadose zone. The choice of which source to model is not important, as long as there is knowledge of the soil vapor concentration near to the condensed phase that is the source of the vapor. Quite often, groundwater contaminant concentration measurements have been used to estimate vapor source strength, using Henry's Law to relate the water concentration to the vapor concentration. This may be tricky, for several reasons. One is that the Henry's Law constant for the contaminant needs to be known, and it is sometimes overlooked that this is a function of temperature. Perhaps more important is the question of what groundwater measurement to use. There may be a significant vertical gradient in concentration within a groundwater source, bearing in mind that the chlorinated solvents of interest in this work are dense non-aqueous phase liquids (DNAPLs) and will tend to sink to the bottom of an aquifer. Diffusion of these contaminants is much slower in water than in air, and there might be limited vertical mixing within an aquifer; the aquifer might receive fresh, relatively clean recharge water from above. Hence, the indiscriminate use of "groundwater concentration data" carries with it the danger of mischaracterizing source strength.

Subject to the above caveat, it is here assumed that the contaminant source is groundwater uniformly underlying the structure of concern. The top of the water table is assumed to be 4 m bgs, and it is infinitely and homogeneously contaminated with TCE, i.e. the groundwater contaminant concentration does not change over time nor are there any concentration gradients within the aquifer. Specification of the actual concentration value in the groundwater source is unnecessary, because whatever choice is made (within reason) all of the calculated results will scale linearly with whatever concentration choice is made.

Since the model being developed is a vadose zone model, it is clear that the properties of the soil between the source and the structure of interest will play an important role in determining transport of the contaminant vapor. Here, the soil is assumed to be homogeneous and be of sandy loam character, using the US Department of Agriculture classification scheme. In the present model, there are no distinct soil layers, rocks, etc. assumed, though these can easily be incorporated, and they can have important effects [46]. It is also assumed that no contaminant adsorption occurs into/onto the soil. This will be discussed at some length further below, but for the moment it is unimportant because of the assumption of a steady state model. This is because at every position in the soil the concentration of contaminant vapor is steady (unchanging with time) and thus at every position the soil in contact with that vapor has come to steady state with respect to the local concentration. This means that there can be no net flux due to adsorption or desorption from the soil phase, and this transport mechanism does not need to be accounted for. The situation changes when unsteady state transport is of concern.

For performing the vadose zone transport calculations around a structure, it is necessary to consider how large an area needs to be included. In other words, for a 10 m x 10 m house footprint, how far from the house will the existence of open soil make a difference in the calculation? This question has been examined in earlier work using such models, and the conclusion is that modeling the vadose zone transport to a distance of 10 m from the structure is generally sufficient [46]. Thus, here, the assumption is made that the house is surrounded by open ground that extends 10 m from the foundation wall. It will be shown that at distances of but a few meters from the structure's foundation the transport of contaminant vapor from the source is not influenced by any advection driven by pressure gradients created by the structure- it is purely determined by steady state diffusion.

In this case, assuming a uniform soil, if the role of soil moisture were to be neglected (discussed below) the concentration gradient from groundwater source to the atmospheric sink above the ground surface would be linear.

Contaminant vapor concentration in the atmosphere is generally assumed to be so low that it is effectively zero, i.e., contaminant vapors that reach the ground surface are immediately infinitely diluted. This might not always be the case in certain locations, but for most circumstances, this is a reasonable assumption.

The only driving force for possible advection of soil gas is the pressure gradient between the interior of the structure and the soil surrounding the foundation. While there of course exists a pressure gradient with depth within the soil gas, corresponding to the pressure exerted by a column of fluid acted upon by gravity, this is normally neglected in such analyses because this same pressure gradient exists both inside and outside of the structure. The structure's interior is typically assumed to be slightly depressurized relative to ambient due to the “stack effect” already mentioned in the previous section. The pressure differences induced by the stack effect are normally quite small. A typically assumed value of the indoor/outdoor pressure difference is -5 Pa. This pressure difference induces airflow from the ground surface through the soil, and into the structure via the foundation breaches. This airflow interacts with contaminant diffusion in the soil, aiding entry of contaminant into the structure. Figure 2.1 summarizes this scenario. It is understanding the complicated interplay of the diffusion of contaminant from the source with any induced airflow that presents a challenge in making good predictions in VI scenarios.

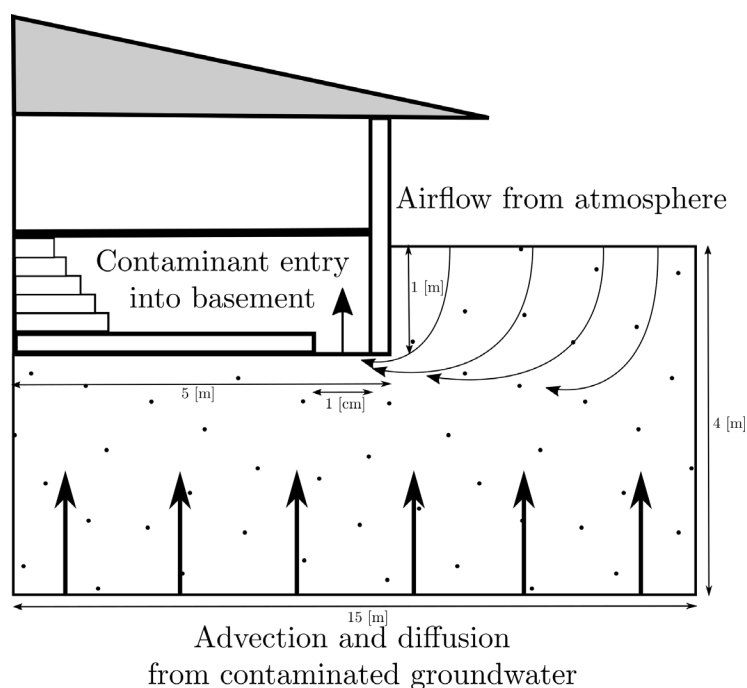


Figure 2.1. The Modeled VI Scenario.

2.3 THE WORKING EQUATIONS

This section outlines the basic working equations that will be more fully developed below. The intent is to first show the key elements of the model, before getting into the details of their implementation. This discussion shows how these equations work together to formally describe the scenario illustrated in Figure 2.1.

Calculation of Indoor Air Concentration

As noted above, the calculation of indoor air contaminant concentration is formally not part of the basic fluid dynamics model of contaminant vapor transport through the vadose zone, which is the main part of the VI model. The indoor air contaminant concentration calculation is something that is performed once the VI model provides an entry rate into the structure. There are those who argue that the entry rate itself is actually the more “fundamental” quantity, since it is not influenced by variations in the indoor air exchange rate. But since comparison of modeling predictions with indoor air contaminant concentration measurements is inevitable, it is necessary to consider how this calculation is performed. Even though it is actually the last calculation performed for a given VI scenario, since it is not part of the rest of the calculations it is presented first.

The indoor volume receiving the intruding contaminant compound (in this case, the basement) is modeled as a well-mixed, or continuously stirred, tank (CST). This “tank” is continuously purged by air taken in from outdoors and exhausted at the same rate to the outdoors. Except in rare circumstances, the air entering from outdoors is free of contaminant. The purge rate is what is termed the air exchange rate, A_e reflecting how many times the air in the volume of interest is exchanged per unit of time (customary units, hr^{-1}). The total molar contaminant entry rate through all of the foundation breaches (cracks) is n_{ck} (moles/hr). If the volume of the intruded space (the basement) is V , then the molar indoor air contaminant concentration in that volume (c_{in}) is simply:

$$c_{in} = \frac{n_{ck}}{VA_e} \quad (2.1)$$

The volumetric contribution of soil gas entry rate (the airflow carrying the contaminant in from below the foundation slab) is usually negligible compared to the air exchange rate with the outdoors, so it is neglected. For typical residential structures, the air exchange rate (through windows, doors, walls, and designed ventilation devices) is of order 1 house volume/hour (see Figure 3.4 below), meaning that the volumetric flow is of order $10^3 \text{ m}^3/\text{hr}$. In contrast to this, the entry rate through a typical crack would only be of order $10^{-2} \text{ m}^3/\text{hr}$ [46], hence neglect of the latter quantity is fully justified. In this equation, since V and A_e are known, the only quantity that is needed to make an estimate of c_{in} is the molar entry rate of contaminant, n_{ck} . The value of n_{ck} comes from modeling the contaminant transport rate in the soil.

The Species Advection-Diffusion Equation

This equation is sometimes termed the “species continuity equation” or the “species convection-diffusion equation”. The general form of this equation is:

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\mathbf{v} c) + R \quad (2.2)$$

where c is the concentration of contaminant vapor at any time and any position in the soil, D is the diffusion coefficient of contaminant in the soil, $\mathbf{v}$ is the velocity field of soil gas, R is a source or sink of the contaminant (as by reaction) and t is time. This advection-diffusion equation is written in a form suitable for describing contaminant vapor species transport in a porous medium, i.e., soils, but because of the possibility (or likelihood) of partitioning of the contaminant species to soil particles or to moisture in the soil, the bookkeeping can become even more complicated than this equation suggests. However, as already noted, these complications are not needed in the steady state representation of the VI problem, and the time derivative of c is also zero, greatly simplifying the analysis.

The contaminant transport itself is driven by both a concentration gradient (leading to diffusive transport, reflected by the term involving the diffusivity D) and airflow (leading to advective transport, shown by the term involving the velocity of soil gas flow $\mathbf{v}$) in the soil. Application of this equation at the boundary of the soil domain, i.e., the foundation breach, provides the value of n_{ck} needed for estimating the indoor air contaminant concentration.

For petroleum-derived volatile compounds, the reaction term R can be important (due to biodegradation processes) but in chlorinated solvent VI, that term can generally be neglected. It may be seen that if R is neglected, and the diffusivity is a known physical property of contaminant in the soil air spaces, then at steady state the only thing not known a priori, which is needed for solving the equation, is the soil gas velocity field $\mathbf{v}$.

Calculation of Airflow in the Soil

The airflow in the soil, $\mathbf{v}$, is obtained using Darcy's Law for flow of fluids in porous materials. This flow is driven by a pressure gradient in the soil, which induced by the indoor/outdoor pressure difference at the interface between soil and building foundation. The simplest form of Darcy's Law is:

$$\mathbf{v} = -\frac{k}{\mu} \nabla p \quad (2.3)$$

where k is the permeability of the soil (in m^2), μ is the viscosity of the soil gas (air, in Pa-s), p is the local pressure (in Pa) and $\mathbf{v}$ is the local fluid velocity. Thus, once the pressures at the boundaries of the soil domain are specified (i.e., at the ground surface and at the foundation breaches) then the velocity field needed in the advective diffusion equation is known.

One additional aspect of the typical VI situation is that the concentration of contaminant in the soil gas is so low that the solution of Darcy's Law is possible without considering the effect of the contaminant on its solution- the flow can be modeled by assuming that soil gas is simply air. This often simplifies solving the VI model, because the solution of Darcy's Law can be carried out first to provide a value of the velocity field $\mathbf{v}$, and then the advection diffusion equation can be solved subject to that known velocity field.

The Role of Soil Moisture

In the above equations, the transport properties of contaminants in soil feature prominently. Both the diffusivity (D) and the permeability (k) appear in the key transport equations. Both can be significantly affected by the presence of liquid water between the soil grains. For example, if the pores in the soil are filled with water, the diffusivity that characterizes contaminant transport in the advective diffusion equation becomes the diffusivity in water instead of in air. The former is several orders of magnitude lower than the latter, which significantly slows the rate at which contaminant can diffuse through the soil. Similarly, if pores are partially water filled, the soil permeability for airflow is much lower than if they are filled with only air. The vadose zone is generally partially saturated with water, even without transients in moisture content that are caused by precipitation. Close to the top of the water table, in the capillary zone, soil pores are partially water-filled. Soil moisture content decreases as a function of elevation above groundwater z [m].

Thus, the soil moisture content θ_w must first be determined in order to solve the contaminant advective diffusive transport equation and Darcy's Law. As a result, the model of contaminant transport in the vadose zone depends upon soil moisture content in a complex way. The choice of how to model moisture profiles in the soil is critical, and sometimes used simplifications to model soil as "dry" except for a thin capillary zone can give misleading results – moisture profiles are continuous in the soil. In this work, the choice has been made to use the van Genuchten representation of soil moisture profiles [54]. Figure 2.2 shows the coupling between the physical processes.

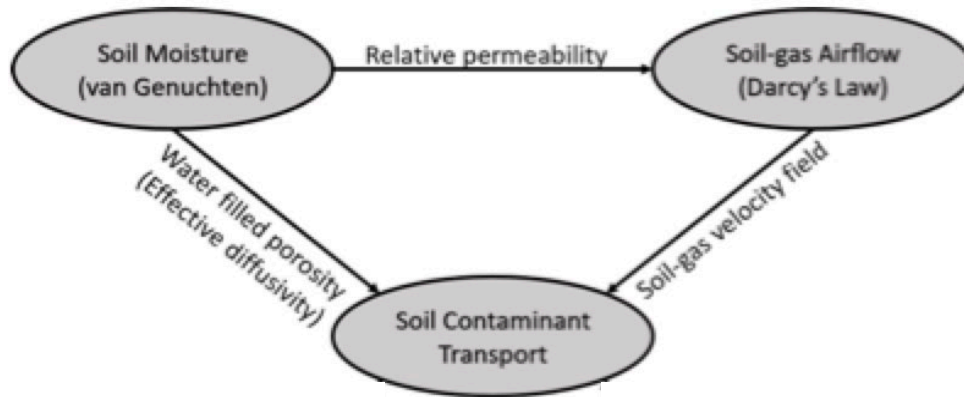


Figure 2.2. The Effect of Soil Moisture on VI Modeling.

2.4 THE FINITE ELEMENT SOLUTION METHOD

Many physical phenomena are described by systems of partial differential equations (PDEs), but for anything but the simplest scenarios, these systems of equations do not have an analytical closed-form solution. This is the case for the partial differential equations presented above used for modeling the VI phenomenon. Therefore, numerical methods are employed for finding approximate, but still accurate, solutions. This involves discretizing the problem, i.e., transforming the continuous problem represented by the PDEs into a series of discrete equations which approximate the PDEs, but which can be simultaneously solved.

There are numerous ways to discretize a problem, and some of the more popular schemes are the finite difference method (FDM), the finite volume method (FVM), and the finite element method (FEM). It cannot be stated that any one method is “better” than the others, but there are certain features that may make use of one method easier in certain circumstances. The three-dimensional equations describing vadose zone transport in VI modeling have been successfully solved using a finite difference solution technique [45]. Here, the choice is made to use the finite element method mainly because of the availability of commercial software packages that eliminate the effort involved in programming the solution using a finite difference method. While perhaps not as straightforward as using common spreadsheet programming tools, employing the commercial FEM packages begin to approach this ideal by allowing the user to select from pre-programmed equations, such as are of interest here, and the software package then does much of the setup work for solution. This will be described in more detail below.

The FEM involves subdividing the domain over which the PDE represented problem is to be solved into many smaller subdomains called elements. These elements can take a wide variety of shapes, e.g., tetrahedra, prisms, or cuboids for three-dimensional problems and triangles or rectangles for two-dimensional problems. The collection of elements that make up the domain or geometry is called a mesh, because when drawn the domain looks like the mesh of a net. The fineness of the mesh, i.e., how small each element within the mesh is, largely determines the accuracy of the solution. Finer meshes with more elements are generally more likely to give accurate representations of the true solution to the PDEs, but increasing the number of mesh elements also increases the computational costs (time) because the finite representation equations need to be solved at each mesh element.

The elements in a mesh can be of different sizes, a fact which allows easier discretizing of complicated geometries. This is analogous to laying floor tiles- the smaller each tile element, the easier it is to make them “fit” around complicated shapes in the floor. This is advantageous for modeling VI, where different parts of the domain have dramatically different resolution requirements. Representing the 1 cm foundation crack requires elements on the scale of mm, while in other parts of the domain, e.g. far from the building of interest, the resolution requirement is on the scale of m. The ability to easily represent complicated geometries with elements of non-uniform sizes helps maintain accuracy while saving computational resources. Another benefit of using these elements is that it is easy to assign different values to physical properties throughout the domain, and thus heterogeneous materials (in this case, soils) can easily be represented. This is important, for example, when dealing with the variation of soil moisture content and its impact on diffusivity and permeability.

A full exposition of the finite element method is beyond the scope of this report, but there exists a wide body of literature on the FEM, and in this work *The Finite Element Method: Theory, Implementation and Applications* [59] has been used as a primary reference.

Aspects Determining the Quality of Finite Element Solutions

The quality of the approximated solution is directly related to the fineness of the discretization (in space, and for transient solutions, also in time). Another aspect that helps determine the quality of the approximated solution is the choice of a *basis function*. If the function u is the exact solution to a PDE over a certain interval I , then this solution u can then be approximated by u_h

$$u \approx u_h \quad (2.4)$$

where u_h is a linear combination of basis functions and their respective nodal coefficients.

$$u_h = \sum_i^n u_i \psi_i \quad (2.5)$$

over I from x_0 to x_n , $i=0,1,2,3,\dots,n$

where u_i is a nodal coefficient; ψ_i is a basis function and where x_0 and x_n are the end nodes of the interval I . The purpose of the basis functions is that they transform a continuous PDE problem into a discrete one. Again, the reader is referred to *The Finite Element Method: Theory, Implementation and Applications* [59] for details. What matters is that the discretization results in a linear system of equations that may be solved to find all of the nodal coefficients u_i . A wide variety of basis functions may be used, but simple ones are usually chosen, e.g. a "hat" functions or some lower-order polynomial, but it is not restricted to these.

An example of an approximation to an exact solution u by u_h as a linear combination of "hat" basis functions can be seen in Figure 2.3. The combination basis functions ψ_i with their respective nodal coefficients u_i gives u_h which gives a piece-wise linear approximation of u . This also shows why basis functions are often called interpolation functions - they can be used to find the value of u_h between nodes. The choice of basis functions in FEM will affect the quality of the solution.

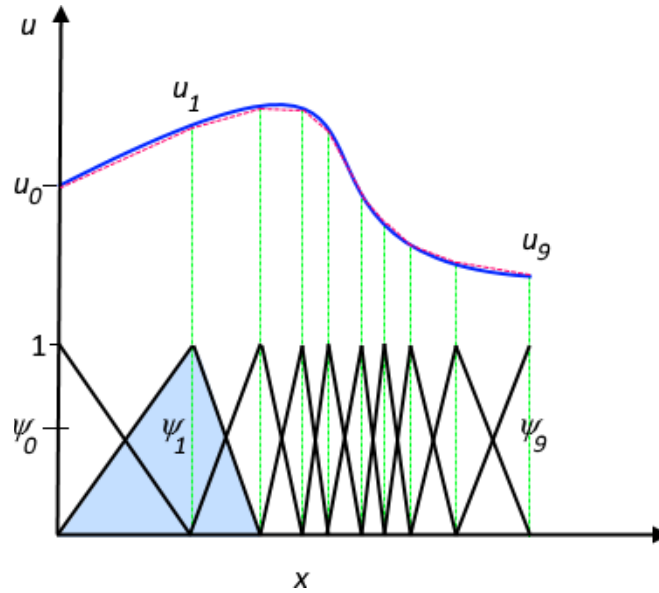


Figure 2.3. The Exact Solution u to Some PDE (Blue Line) and Its Approximate Solution u_h (Dashed Red Line).

The "hat" basis functions ψ_i (black lines) for each element of the interval. The green lines only indicate how the peaks of the basis functions correspond to different sections of the piecewise constructed approximate solution. The combination of each nodal coefficient u_i and basis function ψ_i form the piecewise linear approximation u_h of u . Figure taken from COMSOL.

Using a higher-order basis functions can be much more computationally expensive, and thus typically simple ones are favored - such as hat functions or second order polynomials. The fineness of the mesh becomes more important with simpler basis functions, and becomes the primary means for improving the solution quality. However, there are circumstances when increasing mesh fineness is impossible, and in such cases choosing a higher-order basis function may be the only way to improve the quality of the approximation instead.

2.5 AN EXAMPLE OF SETTING UP A FINITE ELEMENT SOLUTION OF A VI MODEL

As noted above, the intent in this project was to provide a method that allows users who are new to numerical modeling of VI a simple-to-use tool for this purpose. Consequently, the decision was made early on to base the modeling on a commercial platform, in order to make as much use as possible of pre-programmed aspects of a solver. For this reason, a commercial FEM software package called COMSOL Multiphysics was used. There are other FEM solver packages that could be used for the same purpose, but in examining different competitors, it appeared that this was one of the more general, and still user-friendly, packages.

Subsequent sections will cover the steps required to implement a VI model in COMSOL. The steps that will be described include:

1. Creation of the model geometry.
2. Defining the governing equations, boundary, and initial conditions.
3. Discretizing/meshing the geometry.
4. Configuring the solver
5. Post-processing the results.

2.5.1 Geometry Generation

Defining a suitable domain is critical as it determines the computational resources necessary for solving the problem. As noted in Section 2.2, there is a need to include a large enough soil domain around the structure of interest so that the true three-dimensionality of the transport can be accurately represented, while at the same time not needlessly adding areas far from the structure in which the computations will offer no extra insight. Once the size of the domain is selected, the key features must be represented in a drawing that defines the boundaries and/or surfaces of the domain, or features within the domain. An example of the latter is the foundation boundary, which is a central feature of the model. In terms of the example structure illustrated in Figure 2.1, the modeling domain includes everything between ground surface and the water table, but leaving out all interior details of the structure (i.e., the modeling stops at the outside of the foundation wall and bottom of the foundation slab). The domain also extends 10 m beyond the outside of the foundation wall. It is all of these surfaces and boundaries that need to be accurately captured in a drawing of the domain.

The above process may be termed “geometry generation”, which simply means that a drawing is made (within COMSOL) that precisely defines where boundaries and objects exist.

This should be done as accurately as possible while avoiding unnecessary fine details. For example, if a foundation crack is known to have a variable width or slightly irregular shape, it needs to be considered whether this will really impact the predictions (as already noted, it is not likely to do so, as long as the total area open to the soil is represented). Trying to unnecessarily capture very small details will require a fine mesh to resolve, and this becomes computationally “expensive” in terms of computer memory and/or computational time to solve. What is small enough to neglect might not be immediately apparent, so the general approach is to begin with calculations on a simplified geometry whose results can point to where the addition of finer details is warranted. It will be reiterated that the results obtained will not overly sensitive to the nature and position of the actual foundation breach so much as the total breach area [56], so the fact that the example to be presented assumes a perimeter crack rather than some other geometry for the foundation breach is not of great concern.

Another useful feature that allows solution of larger problems with less effort than might otherwise be required involves leveraging symmetry. When setting up a computation, it may be recognized that the two halves of a structure are identical, and that solving the necessary equations for one half of the house is all that is needed. The plan view of the structure that is the subject of analysis in the example to be developed is shown in Figure 2.4. Because the house has a square 10 m by 10 m footprint, the domain actually has two planes of symmetry, which means that modeling any one-quarter of the domain will be sufficient to obtain the solution for the entire domain.

Typically, the geometrical configuration to be modeled is constructed outside of the finite element solver package using computer assisted design (CAD) software. Such CAD packages are often easier to use than the somewhat limited drawing tools within COMSOL but this is not absolutely necessary. If a CAD package is employed, it is possible to import the drawings into the COMSOL package. COMSOL does have a built-in geometry generation tool, which allows the construction of advanced geometries by performing various addition and subtraction operations on simpler pre-programmed geometries.

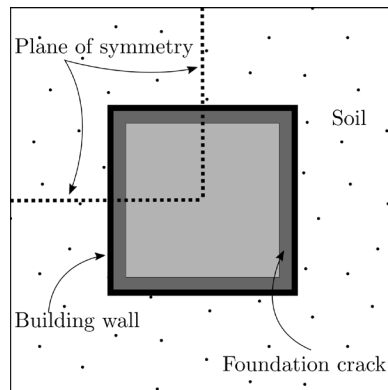


Figure 2.4. Birds-eye View of the Example VI Scenario, Showing the Foundation and the Breach (Crack), Building Wall, As Well As the Two Planes of Symmetry that Allow Representing the Situation by Modeling Only the One Quarter of the Domain.

Only the soil surrounding the structure is the subject of the VI transport analysis, and the interest is in how fast the contaminant enters the structure from the soil. The interior of the structure is not modeled except in the last step of modeling when indoor air contaminant concentration is

calculated from the calculated entry rate and assumptions regarding the impacted volume. The structure is coupled to the modeled soil domain through the foundation crack boundary. Figure 2.5 illustrates the domain that is actually modeled. Note that the foundation and house have “disappeared” because they are not part of the contaminant soil transport calculation. While not visible on the scale of the drawing in Figure 2.5, the crack through which contaminant entry takes place runs along the outer two edges of the foundation cutout. Figure 2.5 has already taken advantage of the two planes of symmetry in the model, and it represents only one of the identical 4 corners of the house. This reduces the number of required mesh elements by 75% as compared with modeling the full domain, which represents a significant savings with regard to computer memory and computation time, with no loss of accuracy. If the structure in question did not have such planes of symmetry, the full domain around the structure would still need to be modeled.

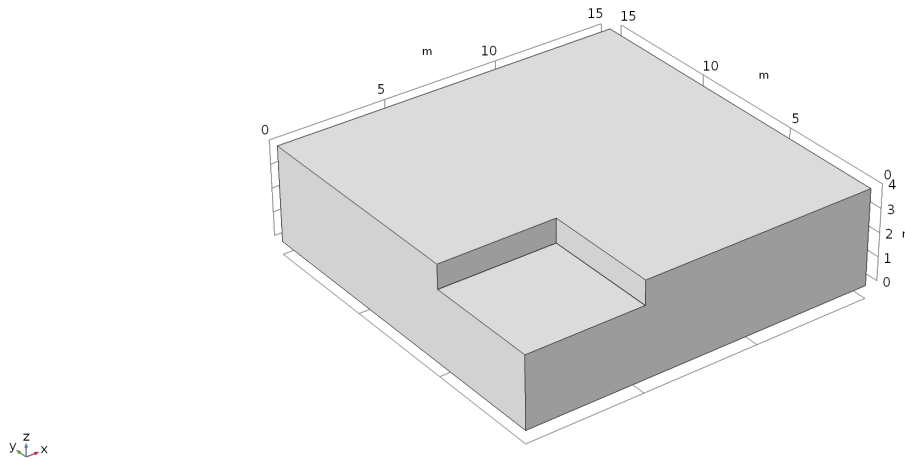


Figure 2.5. The Complete Geometry of the VI Scenario As Implemented in COMSOL.

The actual steps needed to create in COMSOL the geometry shown in Figure 2.5 are described in the Appendix to this report.

2.5.2 Defining the Governing Equations

Throughout this section the books *Contaminant Hydrogeology* [60] and *Dynamics of Fluids in Porous Media* [61] are used as sources, especially on topics regarding soil physics and contaminant transport in soils. The COMSOL reference manuals [62, 63] are also used as sources.

The Indoor Environment

Again, the indoor environment is modeled as described in section 2.3 and the information for that calculation comes from solving for the boundary flux of the vadose zone contaminant transport model at the foundation crack. In this example VI model implementation, it is further assumed that there are no indoor sources of the contaminant nor is there any sorption of contaminant to/from any indoor materials. Only one control volume or compartment is considered within the modeled structure (there are VI models that feature multiple coupled compartments [64], but again, that falls outside of the actual vadose zone transport modeling that is of main interest here). Actual indoor air exchange rates can vary quite significantly, and this a significant source of temporal

variability in VI, a topic that will be further explored in the sections below, which consider transient behavior.

Rate of Contaminant Entry into the Building

Contaminant entry rates into the building are the key values to be determined in the modeling since they directly determine the indoor air contaminant concentration. This entry rate depends on both the soil gas velocity through the foundation breach (advective transport) and the contaminant concentration gradient across the breach (as governs diffusive transport), as already discussed in section 2.3. It is important to note that it is generally not possible to say in advance which of these mechanisms, if either, will be dominant. In fact, it is the dominant mode of entry that distinguishes the behavior of some VI sites from that of others, and this is key to determining whether methods such as CPM or ITS will be effective in characterizing the sites.

Figure 2.6 shows the key elements of the calculation of entry rate from the soil. As described in section 2.3, the key variable to be determined is n_{ck} . But it is immediately apparent that this molar contaminant entry rate may be locally different at different points along the crack that is being modeled. The transport equations that are being solved at the entrance to the crack give the local contaminant flux, j_{ck} . The contaminant entry n_{ck} is given by integrating the contaminant entry flux j_{ck} over the entire area of the crack.

$$n_{ck} = \int_{\text{Total crack area}} j_{ck} dA \quad (2.6)$$

Figure 2.6. Soil-gas Contaminant Vapors Are Transported from the Underlying Soil into a Building Via a Breach in the Foundation.

The scale of the crack is exaggerated. Also, the equations for j_{ck} are approximations to equation (2.10).

The contaminant flux through the foundation crack is modeled as transport between two parallel plates and has an advective and a diffusive component.

$$j_{ck} = j_{\text{advection}} + j_{\text{diffusion}} \quad (2.7)$$

Figure 2.6 shows the usual situation of $u_{ck} > 0$ in which the advective flow is into the house because the interior of the house is slightly depressurized relative to the surroundings. In that case, the diffusive transport and the advective transport both occur in the same direction. On the other hand, if the structure is deliberately over-pressurized, as a result of the normal operation of the HVAC system, or as part of CPM testing, $u_{ck} < 0$ and the advective flow is out of the crack [eg., 17]. In this case, advective flow opposes diffusion. It cannot automatically be assumed, as is sometimes done, that entry of contaminant from the subsurface is totally precluded in that case, because it depends upon the relative magnitude of the advective flow compared to the diffusion driving force.

The flux through the crack is thus calculable from:

$$j_{ck} = v_c c - D^{\text{air}} \nabla c \quad (2.8)$$

here $D^{\text{air}} = 7.2 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ is the diffusion coefficient of TCE in air as the sample contaminant of interest (other contaminant of common concern have comparable diffusivities). The flow through the crack is only in one direction, so the del operator becomes an ordinary derivative, and the velocity vector is resolved into its single component in the direction into the crack (u_{ck}):

$$j_{ck} = u_{ck} c - D^{\text{air}} \frac{dc}{dz} \quad (2.9)$$

This differential equation can be solved subject to the boundary conditions

$$c = c_{in} \text{ at } z = L \text{ (This is the indoor air contaminant concentration, in mol/m}^3\text{)}$$

and

$$c = c_{ck} \text{ at } z = 0 \text{ (the contaminant concentration in subslab soil gas, right at the entrance to the crack).}$$

$$L = 15 \text{ cm is a typical thickness of a foundation slab.}$$

It is easily shown by integration of equation (2.9) that the actual contaminant entry rate is:

$$j_{ck} = u_{ck} \cdot \frac{\exp\left(\frac{u_{ck} L}{D}\right) \cdot c_{ck} - c_{in}}{\exp\left(\frac{u_{ck} L}{D}\right) - 1} \quad (2.10)$$

Here, the superscript “air” has been dropped from the diffusivity D , as it is understood that what is being discussed is the diffusivity of TCE in air. The quantity appearing in the exponential term is the Péclet number for mass transport. It represents the ratio of advective transport rate to diffusive transport. This quantity will be examined in more detail later in this report. It may be

shown, by applying L'Hopital's rule to the above expression, that when $u_{ck}=0$, the expected result of a diffusion dominated result obtains:

$$j_{ck} = D \frac{(c_{ck} - c_{in})}{L} \quad (2.11)$$

The other limit of large Péclet number, corresponding to advective transport control of contaminant entry, leads to the expected limiting result:

$$j_{ck} = u_{ck} c_{ck} \quad (2.12)$$

Without advance knowledge of u_{ck} , it is impossible to know which, if either, limit applies. The solution of Darcy's Law in the vicinity of the crack is thus essential to prediction of what might control the contaminant entry rate into the structure. Again, advective transport through the slab can occur in both directions, i.e. contaminants can be carried from the structure into the soil, under conditions in which the structure is positively pressurized relative to its surroundings [17].

Note that it is not correct to represent j_{ck} as a simple linear combination of these two limiting cases, i.e.,

$$j_{ck} \neq u_{ck} c_{ck} + D \frac{(c_{ck} - c_{in})}{L} \quad (2.13)$$

This may easily be demonstrated if the Péclet number is chosen to be unity and the indoor concentration $c_{in}=0$. In that case, $u_{ck} = D/L$, and the above expression gives a value of $j_{ck} = 2 u_{ck} c_{ck}$, which differs from the correct value of $j_{ck} = 1.58 u_{ck} c_{ck}$.

It is apparent that the contaminant entry rate is thus a function of a quantity that needs to be solved for from Darcy's Law (u_{ck}) but also depends upon the still unknown concentrations (c_{ck} and c_{in}). These are all quantities that are to be determined by solving the equations governing soil gas and contaminant transport in the vadose zone soil domain.

Soil Transport Properties

The rate of transport of soil gas and contaminant through the vadose zone soil will depend upon a combination of a pressure driving force and a diffusive driving force. Since the gas between soil particles consists mainly of air (the contaminant concentrations of concern being typically much less than a percent by volume) there is no diffusive driving force for movement of air in the vadose zone. Instead, the flow is entirely governed by pressure gradients, as described by Darcy's Law. As already noted, the pressure boundary conditions in a VI scenario are normally known or specified. In particular, the pressure at the crack is taken to be the building's indoor air pressure (if desired, the pressure drop for flow through the crack could be taken into account, but this level of detail is generally not warranted). The soil gas (air) flow rate is then determined using Darcy's Law by specifying the value k , the soil permeability in units of m^2 . This is a property of the type of soil (e.g., sand, clay) and its local moisture content. If a portion of the porosity between soil

particles potentially available for airflow is instead blocked by water, the permeability of the soil is much lower than when it is dry.

Likewise the diffusivity of the contaminant in the soil depends upon how much of the potential diffusive pathway is open (air-filled) vs. water filled. The diffusivity of contaminant vapor in air is orders of magnitude higher than the diffusivity of dissolved contaminant in water, so soil pores that are filled with water are effectively blocked as far as diffusion is concerned, and the overall diffusivity of the soil is reduced by a corresponding amount.

The soil between the top of the water table and the ground surface is variably saturated with water. Upward water filling of soil pores from the water table surface is driven by a negative pressure gradient induced by surface tension, leading to a capillary potential. The capillary potential is a function of the soil moisture content and is zero when the soil matrix is saturated with water. The capillary potential varies with the hydraulic properties of specific soil types. Acting counter to the capillary potential is gravitational potential. The water can rise only to a height above the water table at which the capillary potential becomes less than the gravitational potential acting to draw the water back down towards the surface of the groundwater.

There are two common methods for modeling the capillary potential, one developed by Brooks and Corey [65], and another by van Genuchten [54]. Both of these are semi-empirical approaches and rely on experimentally determined parameters for a specific soil type. In this work, van Genuchten's method is employed. Parameters for a wide variety of soils have been made available by the EPA (Table B.1).

The degree of local saturation of soil porosity by water is given by the expression:

$$Se = \frac{1}{[1 + (\alpha h)^n]^m} \quad (2.14)$$

Where Se represents a fractional approach to water saturation of the porosity in the soil, h is the height above groundwater, and α , n , and m are soil-specific parameters, in which $n = (1-m)^{-1}$. It is important to note that $Se = 0$ does not mean that there is no moisture in the soil; soils normally retain a small amount of water termed residual moisture (θ_r).

The total fractional soil porosity available for gas flow or gas diffusion (θ_g) is given by:

$$\theta_g = \theta_t - \theta_w \quad (2.15)$$

where θ_w is the volumetric soil moisture content; θ_t is the total soil porosity. The soil moisture content is related to the saturation value by:

$$\theta_w = \theta_r + Se(\theta_t - \theta_r) \quad (2.16)$$

An example of soil saturation and moisture content as a function of height above groundwater is shown in Figure 2.7 for sand and clay soils.

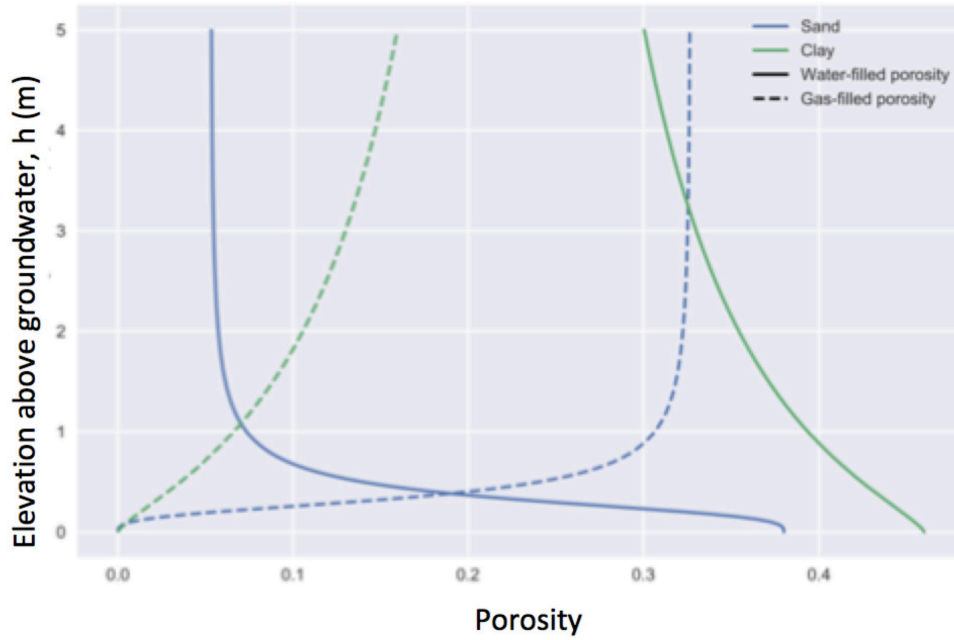


Figure 2.7. The Van Genuchten Soil Moisture Retention Curve, Showing Water Filled vs. Gas Filled Porosity.

The top of the water table is at $h=0$.

It is immediately apparent from Figure 2.7 that sand shows a very narrow capillary zone, in which there is a steep decline in moisture content over some tens of cm above the top of the water table. In contrast to this, clay soil shows a much less well-defined capillary zone, and the part of porosity that is gas-filled is much lower up to several meters above the water table. This means that as compared with sand, transport by both advection and diffusion in clay will be much more restricted. Also, the resistance to diffusive transport of contaminant vapor will be very high in the capillary zone as compared to in the rest of the vadose zone (the difference being much more dramatic in the case of sand). The actual permeability, $k(h)$, for airflow at different points the soil is given in terms of a relative permeability (k_r):

$$k(h) = k_r(h) \cdot k_d \quad (2.17)$$

In which k_d is the dry soil permeability. The relative permeability is obtained from the van Genuchten relations:

$$k_r = (1 - Se)^{0.5} (1 - Se^{1/m})^{2m} \quad (2.18)$$

The variation of permeability with height above the water table is illustrated for typical sand and clay soils in Figure 2.8, in which the values are scaled to the permeability of the respective dry soil, which for sand is almost two orders of magnitude greater than that for clay. It may be observed that for sand, while there is a very significant resistance to airflow in the capillary zone immediately above the water table, within tens of centimeters, the soil permeability reaches a value characteristic of dry soil. The values in clay soil are significantly lower than those in sand throughout the zone, but they qualitatively show the same very significant resistance to airflow near the top of the water table.

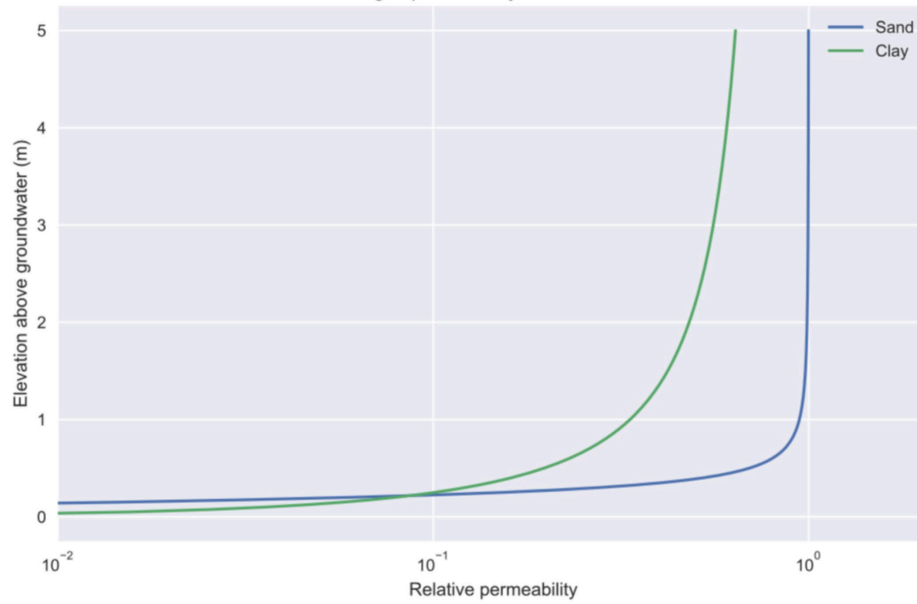


Figure 2.8. The Van Genuchten Relative Permeabilities of Soils to Air Transport.

Note that the underlying permeability of clay is almost two orders of magnitude lower than that of sand.

The diffusivity of the contaminant species in soil is also influenced by soil moisture content. Due to the irregular shapes of pores, diffusion of a chemical species will inevitably often occur along a tortuous path. As this tortuosity depends on the structure of the porous matrix, it is difficult to accurately portray in any detail. A useful empirical approach to approximating this situation was developed by Millington and Quirk [44]. This approach defines an effective diffusivity (D_{eff}) for vapor transport in soil that is represented by:

$$D_{eff} = \frac{D_w}{K_H} \frac{\theta_w^{10/3}}{\theta_t^2} + D_g \frac{\theta_g^{10/3}}{\theta_t^2} \quad (2.19)$$

The fractional porosity terms are as defined above, and D_w , D_g represent the diffusivity of contaminant species (in this case TCE) in water and air, respectively. The constant K_H is the Henry's Law constant for TCE in water. What this expression reflects is the existence of two pathways for diffusion of TCE through the porosity, one through the gas (air) phase and the other through liquid water. As a practical matter, the diffusivity through water is normally several orders of magnitude slower than that through air, so unless there is very little air-filled porosity, the second term will dominate.

Modeling Airflow in the Vadose Zone Domain

It was shown above that the entry rate of contaminant vapor into the structure depends upon the value of n_{ck} , which is calculable from j_{ck} , which in turn depends upon the concentration of contaminant in the sub-slab zone at the foundation crack, c_{ck} . It was also necessary to obtain a value of the flow rate of air in the vicinity of the crack, to establish whether the entry is governed by diffusion or advection or a combination of both. It is the latter quantity that is calculated from application of Darcy's Law in the full soil domain. At steady state, the entry rate of gas from soil into the structure must be balanced by the entry rate of air from the atmosphere into the soil.

This fact has already been illustrated in Figures 1.2 and 2.1. While not considered further here, it is important to recognize that if a structure of interest is surrounded by paving rather than open ground, the path that the air must follow can be quite long, and if the resistance of the soil is high (i.e., permeability low) then this will limit the potential for advective entry. Thus, it is important to correctly model the soil domain to show the source of the airflow into the domain. This will be done in the modeling using appropriate boundary conditions.

This airflow is modeled using Darcy's Law, recognizing that the permeability term in that equation is a function of position, because of the variation of moisture content in the soil of the vadose zone. The general form of Darcy's Law is:

$$\mathbf{v} = -\frac{k}{\mu} \nabla p \quad (2.20)$$

where $\mathbf{v}$ [m s^{-1}] is the airflow velocity vector; k [m^2] is the permeability of the soil, μ [Pa s] is the dynamic viscosity of the soil gas, and ∇p [Pa m^{-1}] is the pressure gradient. This representation of Darcy's Law assumes that the porosity in the soil is filled with the transporting fluid (air), but as discussed above, there is also a second fluid (water) present. However, the water is not flowing, and thus is static, within the pore spaces, and so there is no need to account for its transport. The variation in soil permeability is modeled using the relative permeability expressions from van Genuchten, as presented in the preceding section. The value of k is thus a function of height above the water table (h).

While Darcy's Law relates fluid velocity to a pressure gradient in the vadose zone, obtaining the actual velocity field requires consideration of mass conservation, for which the continuity equation is used. Since for the example calculation steady state is assumed, the continuity equation is simply:

$$\nabla \cdot \rho \mathbf{v} = 0 \quad (2.21)$$

where ρ is the density of the soil gas (assumed essentially incompressible because the pressure variations in these situations are normally so small that they can be neglected). Combining with Darcy's Law, the result is:

$$\nabla \cdot \rho \left(-\frac{k}{\mu} \nabla p \right) = 0 \quad (2.22)$$

where $\rho = 1.225 \text{ kg m}^{-3}$ is the density of air and $\mu = 18.5 \times 10^{-6} \text{ Pa s}$ is the dynamic viscosity of air. Contaminant vapor concentrations are typically very low in VI scenarios, and therefore the contaminant does not affect the density or viscosity of air.

Three boundary conditions are required to fully specify the problem. The first boundary condition is a reference point for where the pressure is zero, at the ground surface boundary from which air is drawn. The second is that the pressure (-5 Pa) at the foundation crack entrance where air exits the soil domain and enters the structure. The third boundary condition is applied to all remaining boundaries in the vadose zone domain, and is a "no flow" boundary condition, indicating that no flow passes through these boundaries. This is true at solid surfaces such as the walls and slab of the foundation, but due to the presence of the symmetry planes used in defining the domain (see Figure 2.4), these planes are also "no flow" boundaries. Summarizing these boundary conditions:

Ground Surface	$p = 0$
Foundation crack entrance	$p = -5 \text{ Pa}$
All remaining boundaries	No flux (i.e., $v = 0$ normal to surface)

Contaminant Transport in the Vadose Zone

In this case, the species continuity equation is utilized as the starting point:

$$\nabla \cdot \mathbf{j} = 0 \quad (2.23)$$

where $\mathbf{j}$ once again is a flux of contaminant (in moles/s-m²). This is simply a statement that in the problem of interest, the contaminant is neither chemically created nor destroyed. This need not always be true, since for petroleum compounds of concern in vapor intrusion, biodegradation can be significant. Such is not the case for the TCE of the model calculation. Just as in considering the entry rate of contaminant into the crack, the flux of contaminant elsewhere in the soil has two components- one associated with advection and the other with diffusion:

$$\mathbf{j} = \mathbf{vc} - D_{eff} \nabla c \quad (2.24)$$

where D_{eff} [m² s⁻¹] is the effective diffusion coefficient of the contaminant in the soil and ∇c [mol m⁻³ m⁻¹] is the concentration gradient. Combining with the species continuity equation:

$$\nabla \cdot (\mathbf{vc}_g - (D_{eff} \nabla c_g)) = 0 \quad (2.25)$$

At this point, with specification of the boundary conditions for contaminant concentration, the problem is ready for solution. The velocity vector comes from solution of the continuity equation with Darcy's Law, as described above. The diffusion coefficient is position dependent, because it depends upon the fraction of porosity that is water filled; the effective diffusivity is higher where there is a greater fraction of air-filled porosity.

Conversion to a water concentration basis

There is, however, an aspect of how the COMSOL solver is set up that requires a few further steps to be taken. These are related to the fact that in the more general case than is considered as an example here, there are other contaminant transport processes that need to be taken into account. Specifically, the contaminant compound can partition into the water phase that is present in the soil, and/or it can adsorb to the surface of soil particles. This has not been considered in a steady state analysis because all of the partitioning processes are assumed to already be in equilibrium, and there is no further partitioning to water or soil particles. All that happens in that steady state case is that the vapor phase contaminant moves through the vadose zone, subject to the equations already derived. But in anticipating the later change to consideration of transient processes, making the change to a basis that accounts for all of the possible processes is useful.

In the general transient case, the total concentration of contaminant at any point in the vadose zone needs to be tracked, as opposed to just the vapor phase concentration that has been the focus so far. This total concentration is given by the sum of the gas, water, and solid phase contaminant concentrations at any given point:

$$c_T = \theta_w c_w + \theta_g c_g + c_s \rho_b \quad (2.26)$$

Here c_T [mol m^{-3}] is the total contaminant concentration at any point in the soil domain, including all possible phases in which it can exist. Some of the contaminant is of course present in the vapor phase (the soil gas) in the air-filled porosity and some is dissolved in the water that exists in part of the pores. The quantities θ_g and θ_w are the gas-filled and water-filled porosities respectively, and c_g and c_w [mol m^{-3}] are the contaminant concentrations in the respective phases. The solid phase sorption contribution has a slightly different form, where c_s [mol kg^{-1}] is the sorbed contaminant concentration per mass of soil and $\rho_b = (1 - \theta_t)\rho$ [kg m^{-3}] is the bulk density of the soil, which can be calculated from the soil porosity θ_t and solid phase density of the soil ρ [kg m^{-3}].

The accounting for the disposition of the contaminant in three phases would appear to make the problem much more complicated, but there are actually simple relationships between the different concentration variables that can simplify the problem once again. At low contaminant concentrations, the gas and liquid phase contaminant concentrations at any point are related through Henry's Law:

$$c_g = K_H c_w \quad (2.27)$$

where, K_H is the dimensionless Henry's Law constant for TCE in water (its value is 0.42 at 20°C [66]). It is typically assumed that there are no temperature gradients throughout the vadose zone, so a single value of K_H applies at all points.

Similarly, the solid phase contaminant concentration can be related to either of the other two concentrations assuming a linear sorption isotherm (as is often appropriate at the low vapor concentrations of interest). Here either the gas-solid or water-solid sorption interaction can be chosen; at present, it is assumed that the available data are in the form of a gas phase partition coefficient, K_p (in m^3/kg) such that $c_s = K_p c_g$.

Thus all contaminant concentrations at any point in the soil matrix can be related to one selected contaminant concentration at that point. Choosing that basic concentration to be the water phase contaminant concentration (c_w), the air phase and solid phase concentrations may be immediately calculated. This focus on water concentration is arbitrary, but commonly utilized. Then the total contaminant concentration at any point in the soil domain can be represented as:

$$c_T = (\theta_w + \theta_g K_H + K_H K_p \rho_b) c_w \quad (2.28)$$

The terms in parentheses are collected as $R = (\theta_w + \theta_g K_H + K_H K_p \rho_b)$ which is commonly called the *retardation factor*. This nomenclature comes about from a common modeling viewpoint in which the motion of contaminants with groundwater is of main interest. Then, the retardation factor indicates by how much the contaminant residence time in the soil matrix is increased compared to the residence time of groundwater, due to transferring between the phases. Again, here, the motion of the groundwater is neglected, so this aspect of transport analysis is not the main focus.

However, the partitioning of contaminant between phases does become important in transient contaminant VI simulations.

Within the vadose zone, advective transport can involve both the water and gas phases inside the soil pores.:

$$j_{adv} = u_{w,pore} c_w \theta_w + u_{g,pore} c_g \theta_g \quad (2.29)$$

Here $u_{w,pore}$ and $u_{g,pore}$ [m s^{-1}] are the water and gas phase *pore* velocities vectors respectively. However, from mass conservation, we know that the product of the pore velocity and porosity is the superficial velocity of a fluid in a porous medium. Combining with Henry's Law gives

$$j_{adv} = (u_w + u_g K_H) c_w \quad (2.31)$$

where now, u_w and u_g [m s^{-1}] are the Darcy or superficial velocity vectors for water and gas flow. But again in the normal analysis of VI, the pore water is considered as immobile, i.e. $u_w = 0$ resulting in:

$$j_{adv} = u_g K_H c_w \quad (2.32)$$

where u_g is the solution obtained from solving Darcy's Law for soil gas, as already presented above. Thus switching to an accounting for water phase concentration, as opposed to gas phase concentration, has changed nothing in the analysis, except to introduce the Henry's Law constant.

It is, however, worthwhile noting that inclusion of transport through pore water motion can be useful if one is concerned about the influence of precipitation on the movement of contaminant vapor [e.g., 52]. To model a scenario where there is a gravitational water potential resulting in groundwater flow, the two-phase Darcy's Law needs to be solved to get both u_g and u_w . This significantly complicates the mass transport aspects and will not be considered further here.

When there is a switch to a water phase contaminant concentration basis, the equation describing diffusive transport of contaminant also needs to be adjusted, and the total diffusive flux through the pore matrix is given by:

$$j_{diff} = -(D_w \theta_w \tau_w \nabla c_w + D_g \theta_g \tau_g \nabla c_g) \quad (2.33)$$

where $D_w = 1.02 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$ and $D_g = 6.87 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ are the contaminant diffusion coefficients of TCE in pure water and air respectively and τ_w and τ_g are constants reflecting the tortuosity of the diffusion path in the soil, and were what was used in deriving the Millington-Quirk effective diffusivity. Thus, the expression for diffusive transport expressed on a water contaminant concentration basis becomes:

$$j_{diff} = -\left(D_w \frac{\theta_w^{10/3}}{\theta_t^2} + D_g \frac{\theta_g^{10/3}}{\theta_t^2} K_H\right) \nabla c_w \quad (2.34)$$

It is immediately apparent that this is the same expression as used for describing the diffusive transport in terms of the vapor phase contaminant concentration, except for the change of variables from gas phase to water phase concentration, using Henry's Law.

This leads to a revised representation of the species continuity equation using the water phase concentration as the locally tracked variable:

$$\nabla \cdot (\nu K_H c_w - (D_w \frac{\theta_w^{10/3}}{\theta_t^2} + D_g \frac{\theta_g^{10/3}}{\theta_t^2} K_H) \nabla c_w) = 0 \quad (2.35)$$

It should be emphasized that there has been no change in the physical nature of the process that is being represented – the only change is in the variable that is used to track the vapor phase concentration, in this case indirectly. The reason for making this change is purely for the convenience of how COMSOL handles the tracking of certain variables, in its pre-programmed equations, and this will be discussed below.

In order to solve this equation, boundary conditions are needed. The boundary conditions may be represented as follows:

At the ground surface $c_g = 0$, or equivalently, $c_w = 0$

At the groundwater surface $c_w = c_{w, source}$

At the foundation crack, flux $= -j_{ck}$

All other solid boundaries – No flow.

The boundary condition at the crack depends upon the local component of velocity into the structure, which is separately obtained from the solution of Darcy's Law for soil gas. It also depends upon the local vapor phase concentration of contaminant at the crack entrance, as well as on the indoor air contaminant concentration. These are coupled equations – c_{in} is obtained from j_{ck} , which is fixed by c_{ck} and c_{in} --this is three equations in three unknowns. Since the representation in COMSOL involves the water phase concentration, it is important to remember that the value of j_{ck} , which is a vapor flux, must be divided by K_H in order to convert it to a water concentration basis for it to be consistent with that representation.

The Importance of Contaminant Diffusivity

Before proceeding to the solution of the above system of equations, it is worthwhile considering one aspect of the model results that will be quickly apparent. Figure 2.9 illustrates how the effective diffusivity, as defined above relative to a water phase concentration, varies from being close to that of the pure water diffusivity near the capillary zone, and increases to something closer to gas-phase diffusivity as the soil moisture decreases going up towards the ground surface. The dramatic difference in these diffusivities is illustrated by the fact that the effective diffusivity is shown plotted on a logarithmic scale. The implication is, as noted above, that when there is even a small amount of air-filled porosity, diffusive transport of contaminant through the air-filled porosity will be much faster than through the water filled pores.

A second implication of the results in Figure 2.9 is that the portion of the vadose zone in what is normally considered the capillary fringe right above the water table represents a very significant resistance to transport of contaminant. In that zone, since porosity is largely water-filled, there will be no advective transport of contaminant (it is also normally quite far from where the pressure driving force for advection is applied at the foundation boundary). Diffusive transport is also very slow, since it occurs mainly through a water phase. It has been shown in earlier modeling work that neglect of this diffusive resistance can lead to important errors in predicting the concentration profiles in the vadose zone [53,67].

The capillary zone resistance may also be significant in the use of groundwater sampling to establish the strength of the VI vapor source, as is commonly done. It is customary to use a Henry's Law constant to convert the measured groundwater concentration to a vapor source concentration, assuming equilibrium at an air-water interface which is taken to exist at the water table. The complexity of the situation in the capillary zone can, however, make this assumption problematic. If the capillary zone is not well-mixed with the underlying groundwater, the capillary zone will represent a significant resistance to the vapors that are released at the water table. This is on top of the question regarding the depth at which groundwater sampling is performed, and whether that sample truly reflects the top layer of water in the water table, which is assumed to serve as the vapor source.

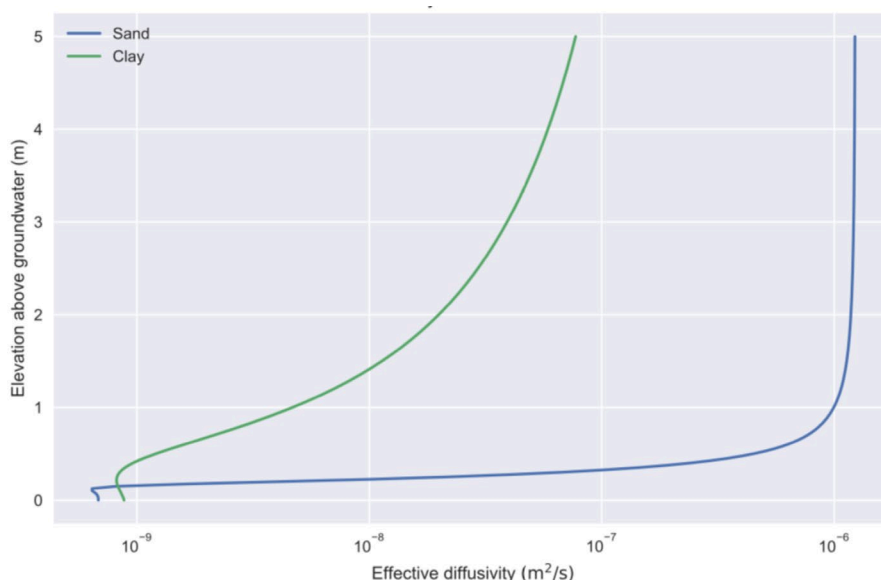


Figure 2.9. Effective Diffusivity of TCE in the Vadose Zone Using the Millington- Quirk Model.

Soil water and gas filled porosities are calculated using van Genuchten's equations.

The Sequence of Calculations

The sequence of calculations is summarized in Figure 2.10. In this figure are indicated the calculations needed to provide the soil gas velocity field and separately from those, the contaminant diffusion and advection, which allows the calculation of entry rate and from that, the indoor air contaminant concentration. The diagram suggests a calculation that is iterated, but in fact, the whole system of equations may be solved in a coupled fashion, as discussed below.

This is the reason that the arrows between the Darcy's Law block and the species continuity block are shown as double headed arrows. In a truly serial calculation, once Darcy's Law is solved, the value of velocity is passed to the species continuity calculation, and there is no need to iterate with Darcy's Law. This will be the basis of the segregated solver approach discussed below.

The intent of the diagram is to show how the different equations fit together to provide the desired predictions. The dashed portion of the diagram is intended to illustrate what might be considered the more logical representation of the process, in which it is the vapor phase contaminant concentration that is directly tracked. The fully equivalent water phase concentration process is shown on the right side of the diagram, and represents the easier way to set up the contaminant accounting in COMSOL. Both approaches are entirely equivalent. The arrow connecting the indoor air concentration back to the species continuity equation reflects the iterative nature of the solution, bearing in mind that the entry rate depends upon the value of the indoor air contaminant concentration. This is because the indoor air contaminant concentration defines the value of the subslab to indoor air concentration gradient governing diffusion entry rate; the higher the indoor air contaminant concentration, the smaller the gradient and thus the lower the entry rate via this mechanism. If diffusion were always negligible (which it is not) then this iteration would not be necessary.

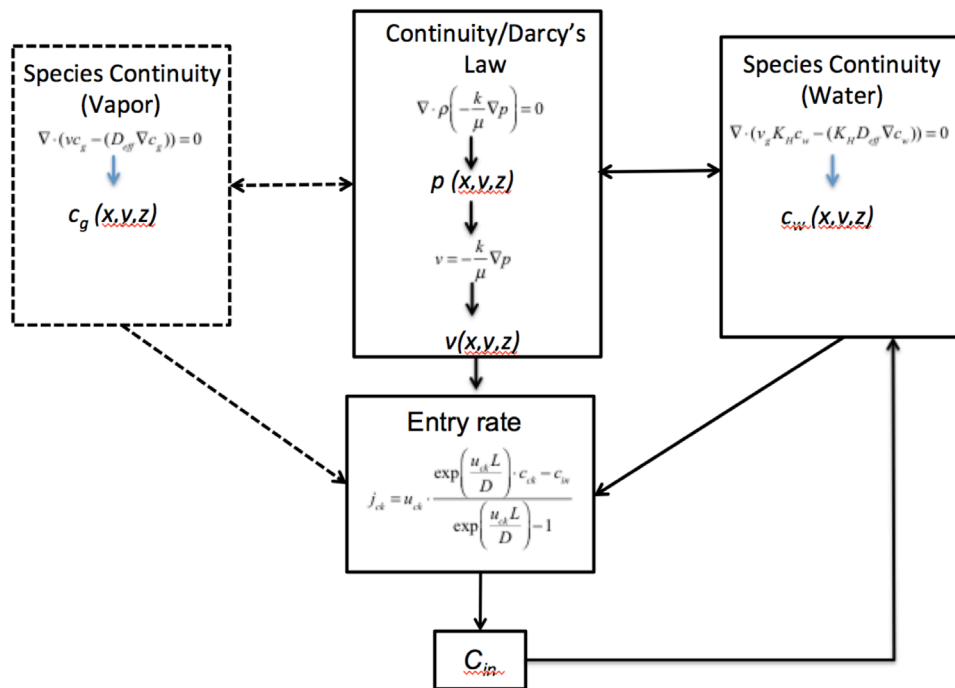


Figure 2.10. The General Calculational Scheme for a Steady State Vapor Intrusion Model.

The dashed lines indicate an alternative calculational sequence to that based on the species continuity equation based on water.

2.5.3 Implementation in COMSOL

In this section, the different steps needed after developing the model equations are illustrated. Since the selected solver is a finite element solver, the concepts of “finite elements” and “meshes” are discussed first.

Meshing

The mesh in a finite element method (FEM) model is the collection of small discrete elements that describe and constitute the model geometry or domain. Meshing is the process of generating a mesh. Meshing is one of the most important aspects of FEM modeling as the mesh directly influences how well the various gradients can be resolved on the mesh. In other words, this determines how accurate the solution can be. Because in the FEM one is modeling continuous partial differential equations by finite “pieces”, the tendency might be to choose as fine a mesh as possible, as that allows the discretization to become closer to the real solution. However, designing a computationally adequate and useful mesh can be challenging, since a finer mesh generally involves a higher computational cost in both memory and computational time. A good mesh designer must constantly balance accuracy against computational costs by considering where a mesh can be finer and where it can be coarser.

The most fundamental units of the mesh are the individual elements that comprise the mesh. There are many different types (shapes, forms) of elements that can be used for meshing and the choice of which to use depends on the spatial dimensionality of the model, the particularities of the geometry, and the nature of the equations that need to be modeled on the mesh. Different element types are needed to model a two-dimensional (2D) problem as opposed to a three-dimensional (3D) geometry. The elements needed for performing a 2D calculation are flat, much like tiles that are used to cover a particular area of a floor. Simple examples are triangular and rectangular shapes, such as illustrated in Figure 2.11. These elements cannot, however, capture what equations that describe 3D phenomena require.

There are primarily four basic types of 3D mesh elements available - the tetrahedral, cuboid, prism, and pyramid (see Figure 2.11). These can be combined in various ways to represent any 3D geometry. The most general 3D element is the tetrahedral shape and it can be used as the basic building block for approximating any geometrical object. However, it is not always the most effective choice for meshing a given geometry and another element type may be better suited. Consider trying to model the laminar flow of a fluid in a pipe. Because of symmetry, only a small wedge of the pipe needs to be explicitly modeled (see Figure 2.12). Therefore, in this scenario, it might be beneficial to use prism elements rather than tetrahedrals, since these are already wedge shaped.

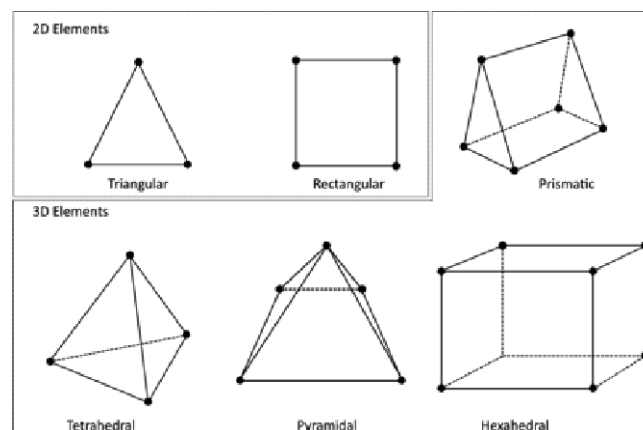


Figure 2.11. Some Common Mesh Elements.

Figure from COMSOL.

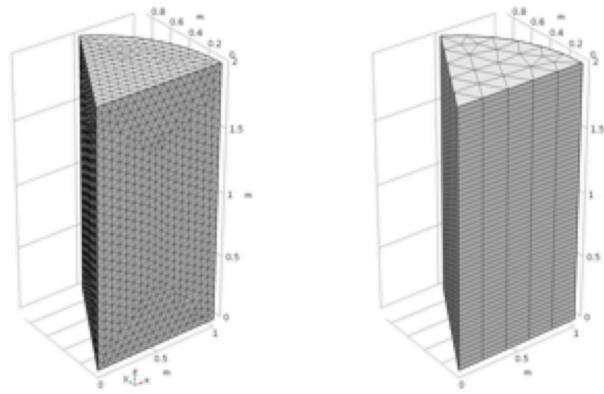


Figure 2.12. By Noting the Symmetry Inherent in the Problem of Laminar Flow in a Pipe (segment), Clever Mesh Design Can Significantly Reduce the Number of Mesh Elements Needed to Describe Gradients (Here Assumed to Be Important in the Axial Direction).

Notice that the mesh density in the axial direction is more or less the same in both implementations.

This is of course a relatively simple example and more complicated geometries may benefit from use of many different kinds of elements. These types of multi-element meshes can give significant computational saving but can require significant user effort to generate. Sticking to one type of element is often simpler as these can be used to quickly and easily mesh geometries.

Meshing can be performed manually, but is often performed using a meshing algorithm. The creation of these algorithms is a science in itself. Their use generally requires passing some basic parameters to the algorithm. For example, the user will often specify the maximum and minimum element sizes, maximum element growth rate (discussed below), and 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 particular interest particularly where there are steep gradients expected. There are also a variety of specialty mesh features such as boundary layer meshes, which add finely spaced mesh layers that parallel a particular boundary. Learning the use of the many meshing tools can be one of the more challenging aspects of FEM modeling.

Meshing the Example VI Model

The first choice to make is that of element type, and the choice is informed by the gradients of the dependent variables. Based upon van Genuchten's moisture retention curves, there will be a large soil moisture gradient in the capillary zone, which will require a relatively fine mesh to be resolved. In other words, where a key variable is changing quickly in value with position, fine meshes and correspondingly small elements are needed. Meanwhile, the airflow calculated from Darcy's Law will give rise to streamlines from the ground surface to the foundation crack and the pressure gradients will be orthogonal to these streamlines. The contaminant concentration gradients will be difficult to predict a priori, but there will certainly be a gradient from the groundwater vapor source to the ground surface and foundation crack. This discussion points to the fact that these different gradients will intersect but be in different directions. Thus, there is no one obvious direction in which to specify fine elements, and it makes sense to specify tetrahedral elements to mesh the geometry. This does not yet indicate the element size or whether the elements need to be fine or can be coarse at any location.

Properly meshing the geometry in the case of a VI domain is a challenge due to the great range of geometric scales of relevance. The house and soil domains are characterized by sizes of order of meters whereas the foundation crack is only 1 cm wide, and requires very fine meshing. This is not only because of its small size, but also because the contaminant entry rate is calculated based on the values of velocity and contaminant concentration here, hence there is need for accuracy of the solution in that area. The need for fine meshing in this location exists regardless of whether contaminant entry is dictated by advection or diffusion, since it is important to get both the velocity and concentration gradients correct at this location.

The domain to be meshed is that shown in Figure 2.5. It needs to be filled in with finite elements over which the different partial differential equations are solved. Once the general considerations for meshing have been decided upon, the simplest approach is to begin with a meshing tool that is inherent in the FEM package itself. The COMSOL meshing algorithm only requires a few parameters to mesh the geometry shown in Figure 2.5 with tetrahedral elements. A description of the parameters and their typical values are given in Table 2.1.

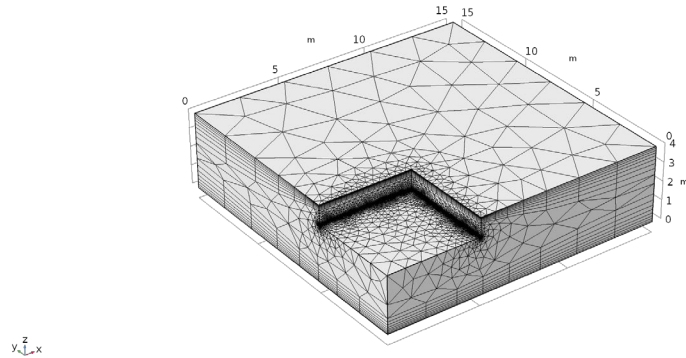
Table 2.1. Inputs to COMSOL's Meshing Algorithm.

Input	Value	Description
Maximum element size	1.5 m	Maximum size of a element
Minimum element size	1 mm	Minimum size of a element
Maximum element growth rate	1.3	Maximum allowed size increase of adjacent elements
		1.3 indicates that an element can only be 30% larger than its neighbor. A smaller value gives a finer mesh.
Curvature factor	0.4	Ratio between the boundary element size and the geometry curvature radius. A smaller value gives a finer mesh.
Resolution of narrow regions	1	Control the number of layers of elements that are created in narrow regions. A larger value gives a finer mesh.

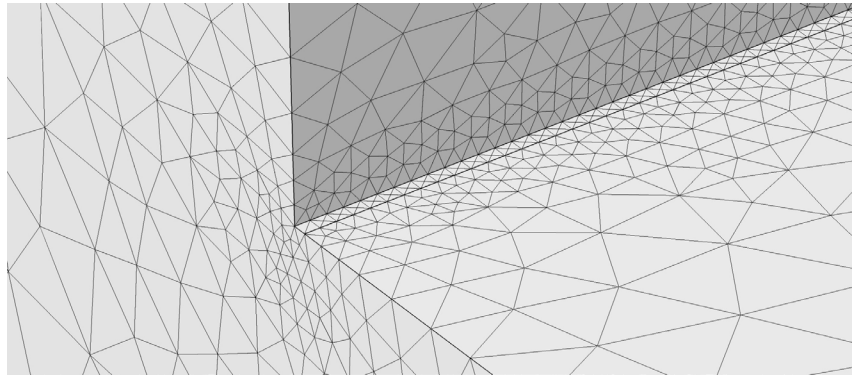
Because the domain is characterized by length scales up to 10 m, meshing the entire domain with tetrahedral elements that were, say, 1 mm in scale, would require a prohibitive number of elements if the solution is to be affected on a desktop computer. This may be crudely estimated by describing the domain as 10 m x 10 m x 4 m; the number of 1 mm elements to fill this volume would crudely be 400 billion, which would be entirely unrealistic as well as unnecessary. Near the edges of the domain, where there are no significant gradients to be expected, the elements can approach the maximum size of 1.5 m each. Working inward from the outer boundaries of the domain, the mesh size is gradually reduced by a factor of 1.3 for each step decrease in element size.

When dealing with steep gradients in one particular direction at boundaries, such as that discussed relative to the capillary fringe, a boundary layer mesh may be employed. This is a type of mesh that is not tetrahedral, but instead introduces a thin mesh layers paralleling the surface a boundary. The number of boundary layers is specified by the user, and in the example case 8 layers are chosen (though more could be added if needed). The thickness of each layer is determined by the size of the other elements in its vicinity, as well as the growth rate parameter, here 1.3. This means that the mesh layer thickness increases by 30% for each added layer. Figure 2.13 shows the mesh that was automatically created using the parameters in Table 2.1 and the choices regarding the boundary layer mesh.

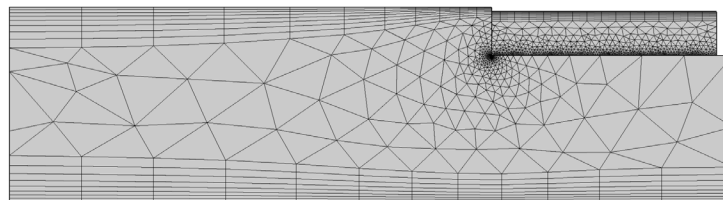
Figure 2.13a shows how the elements decrease in size from the domain boundaries, where no steep gradients of velocity or concentration are expected, to very fine near the entry crack area outside of the foundation. The finer mesh near the crack area is more clearly visible in Figure 2.13b. Note the regularity in decrease in mesh size while approaching the crack area. The use of the boundary layer meshes is visible in Figure 2.13c. This sort of mesh makes sense along the bottom of the domain, since the groundwater source is uniform across the whole domain. Likewise, the ground surface is quite uniform as one moves away from the boundary defined by the foundation wall.



(a) *The darker perimeter around the foundation highlights the higher mesh density along the foundation crack.*



(b) *Close-up of the foundation crack mesh.*



(c) *Side-view highlighting the boundary layer mesh.*

Figure 2.13. Initial Finite Element Mesh for the Modeled Vapor Intrusion Example.

Solver Selection

A solver must be chosen to effect the actual numerical solution of the partial differential equations on the prescribed mesh. The *COMSOL Multiphysics Reference Manual v5.3a* is the basis for this discussion.

The example problem is a steady state problem, which is simpler to implement than a transient solution that introduces time as another independent variable. The VI model as formulated is termed a multiphysics problem in COMSOL, meaning that many of the physical parameters depend on each other, and how to couple them needs to be specified. The parameters can be coupled employing either a *segregated* or *fully coupled* approach. In a segregated solver, each governing equation is solved separately in a specific order. For instance, in the VI example, Darcy's Law can logically be solved first, to obtain a solution for airflow velocities in soil. The obtained velocity field can then be an input into the contaminant transport equation solver. When that solution for concentration profiles is obtained, that can be used to solve the equation governing contaminant entry rate, and following that, the indoor concentration equation can be solved. This means that the calculations are performed in a serial fashion that is iterated until convergence occurs in all of the separated steps. This is necessary because of the coupling between the entry rate and the concentration at the crack. In the case of typical VI calculations, the use of the segregated approach is fully justified because the concentrations of contaminant vapors are normally so low that they have no impact on the solution of soil airflow using Darcy's Law. When solving on a desktop computing system this approach will generally lead to good results without requiring very long computation times.

The alternative to the segregated computational approach is the fully coupled approach, which assembles a single large system of equations all solved at the same time. In effect, the iteration that is somewhat manual in the segregated approach is automatically taken care of in the fully coupled approach. Both the segregated and fully coupled approaches should reach the same solution, but the fully coupled approach will do so faster, but at the expense of using more memory.

Regardless of the coupling assumption, a solver must be specified to actually solve the system of equations. The choice is to use either use a *direct* or an *iterative* solver. Direct solvers, as the name implies, arrive at a solution directly and are based on LU-decomposition (basically a form of Gaussian elimination for solving the system of linear equations used to approximate the solution). Iterative solvers on the other hand, iteratively approach the solution, and are based on the conjugate gradient method. The advantage of direct solvers is that they are faster, but use more memory, while iterative solvers are slower but use less memory. In terms of choosing a solver algorithm, there are many options, but MUMPS (Multifrontal Massively Parallel sparse direct Solver, see <http://mumps.enseeiht.fr>) and GMRES (Generalized Minimum Residual Method, see <https://mathworld.wolfram.com/GeneralizedMinimalResidualMethod.html>; Saad, Y. and Schultz, M. "GMRES: A Generalized Minimal Residual Algorithm for Solving Nonsymmetric Linear Systems." *SIAM J. Sci. Statist. Comput.* **7**, 856-869, 1986) will be used as the respective algorithms for direct and iterative solvers.

For completeness, to solve a transient or time-dependent problem (which will be discussed in a later section) a solver that "steps forward" in time is required. In this case, just as with the meshing of the physical dimensions of the problem, correct choice of the "size" of the time step is critical to obtaining a good solution. Too large a time step causes stability issues and ultimately convergence is impossible.

The choice of some appropriately sized time step is required for a solution to be achievable. A time-dependent solver helps select an appropriate time-step and there are several popular approaches to implementing a solution, such as high-order Runge-Kutta (RK) or the backwards differentiation formula (BDF). Regardless of the type of solver, for each time step the system of equations is solved using one of the aforementioned solvers. The difference between RK and BDF is that RK explicitly discretizes time while BDF does so implicitly.

Again, the choice of solver should not affect the solution to the problem. However, it can have a large impact on computational time and resources, and these considerations will dictate solver choice (the choice is also partially dependent on the mesh, as this will also affect memory usage). In this example, and throughout the models used in this work, the choice was made in favor of speed over memory and therefore the fully coupled approach with direct solvers was adopted. Depending upon the computing equipment that is available, and the scale of the problem to be solved, another approach might sometimes make sense.

Adaptive Mesh Refinement

It has been noted that the accuracy of the solution obtained by the FEM is dependent on the quality of the mesh. While the mesh designer can do much to create a mesh that performs well for the particular problem posed, refinement of the mesh is often needed and should be performed for every new model. What this means is that the solution that is obtained using the first proposed mesh is not immediately accepted as “correct”. In the kind of complicated problem that is being modeled here, there is no real way to judge if the solution that has been obtained is as accurate as possible. One way to judge how good the solution is involves refining the original mesh in light of the solution obtained with that mesh. Fortunately, this can often be done automatically.

There are two types of mesh refinements in the FEM. The first type reduces the size of the elements and thereby increases the accuracy of the solution. This is called *h-type* refinement (*h* is often used to denote the mesh size). The second increases the order of the polynomial used as the basis function, called a *p-type* refinement, which likewise increases the solution accuracy. The *h-type* refinement is generally more attractive because it is simpler and the computational cost of using the *p-type* refinement increase faster than *h-type* refinement. However, *p-type* refinements are useful if the user imports an already existing mesh, and is unable to change it, rendering an *h-type* refinement impossible. These two methods can also be combined to perform an *hp-type* refinement.

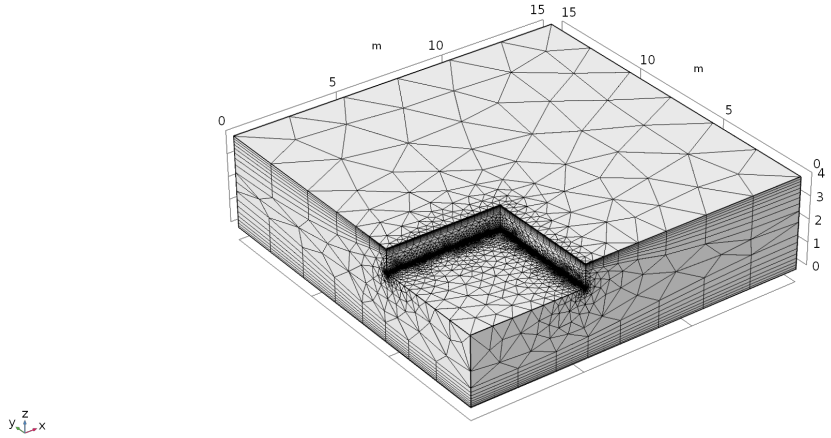
Refinement is usually done on the basis of an algorithm, which is possible because the FEM has a built-in ability to estimate the local error of the solution anywhere in the domain. The downside of using an algorithm built into a package such as COMSOL is that the user has little control over how the mesh is refined. The user can, however, solve the model while the mesh is stepwise manually refined by the user, and plotting what happens to some relevant metric of the solution. This can be very time consuming, and therefore use of algorithms is usually preferable. A hybrid approach is to manually alter the mesh after the algorithmic mesh refinement.

Refinement can either be done locally or globally. Global refinement involves defining some singular metric that will be used to evaluate the quality of the mesh, e.g., indoor air contaminant concentration. In local refinement, one still has to define some metric for evaluating the quality of the refinement, but evaluation only occurs on a subset of the domain, e.g., a local contaminant concentration value.

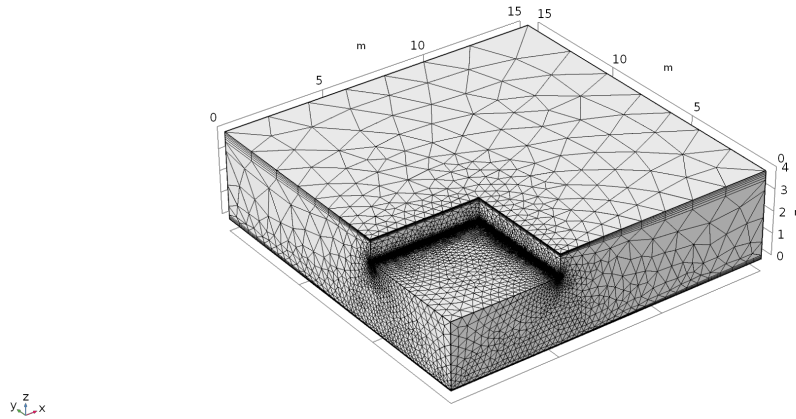
In both approaches elements having the largest estimated local relative error are refined, but the exact details of the refinement can differ between specific refinement algorithms. The local relative error is defined as the difference of the approximated solution u_h from one mesh to another.

$$e = u_{h1} - u_h \quad (2.36)$$

e is the estimated local relative error (for every node); u_{h1} and u_h are the approximated solutions on the refined and original meshes respectively. The optimal type of refinement varies by problem, but a global refinement will generally be more computationally expensive.



(a) Original mesh. 362,657 elements.



(b) Refined mesh after global refinement with respect to the indoor contaminant concentration. 1,065,743 elements.

Figure 2.14. Original and Adaptively Refined Meshes.

In this work a global h-type refinement was adopted and the indoor air contaminant concentration, c_{in} , was the refinement metric. COMSOL's refinement algorithm can actually reinitialize the mesh, and it can thereby coarsen elements, i.e., increase h where the local error is very small. A fine mesh is not needed far away from the foundation crack, but it might not be obvious before beginning calculations where a coarser mesh is acceptable.

Coarsening the mesh where fine detail is not needed saves computational resources. In an illustration example shown here, the algorithm is allowed to refine the mesh four times, and stop if the total number of elements exceed 1 million, with a maximum coarsening factor of 3, and element growth rate of 1.3, i.e., the number of elements can increase by roughly 70% each iteration.

The result of an automated mesh refinement process on the example VI model is shown in Figure 2.14 where the original and refined meshes are juxtaposed. Note that following mesh refinement, the mesh is denser near the foundation, the boundary layers tighter (in particular near the groundwater boundary), and the elements are larger in the periphery of the domain. The original and refined meshes have 362,657 and 1,065,743 elements respectively. Figure 2.15 shows how the estimated value of indoor air contaminant concentration, c_{in} , converges over each iteration of mesh refinement.

What is shown in Figure 2.15 is the change in calculated indoor contaminant concentration with iteration. The first automated refinement did not improve the estimates very much, but with the second refinement very large changes are seen in the error in predicted values. By the 4th iteration, the improvements in the estimates of c_{in} are becoming very small (note that the errors are plotted on a logarithmic scale).

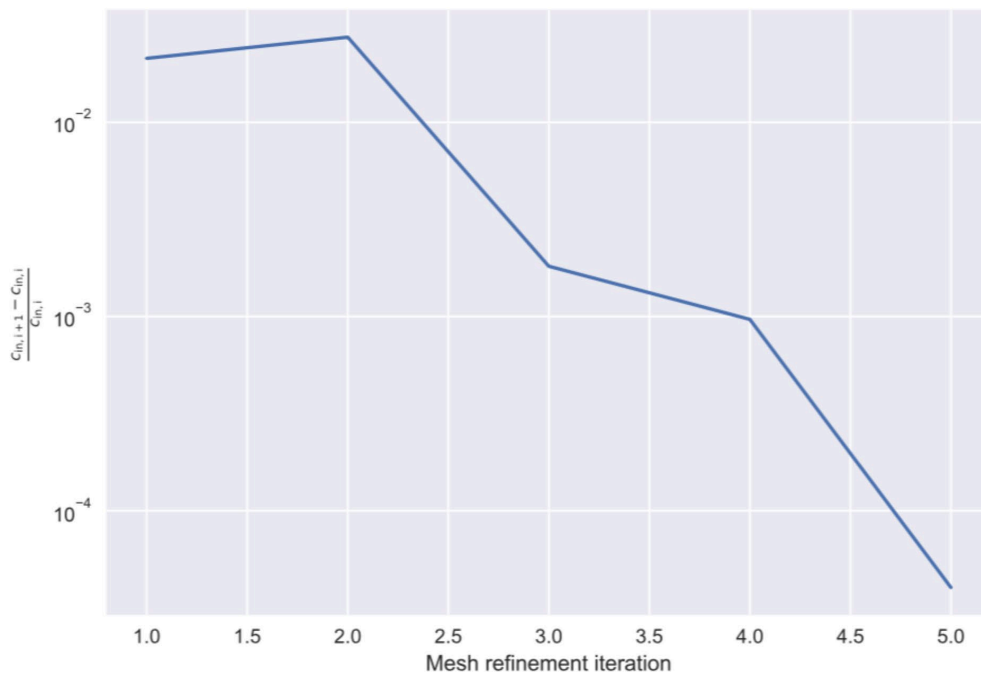


Figure 2.15. Convergence of Indoor Air Contaminant Concentration As the Mesh Is Refined.

Displaying the Results

One of the benefits of using a FEM package such as COMSOL is found in its advanced post-processing capabilities. This allows the user to examine the results driving VI in great detail. For example, Figure 2.16 shows the pressure field in the sample VI problem, obtained by solving Darcy's Law. Also shown are the associated airflow streamlines in the soil domain.

What is pictured in Figure 2.16 is a simple side view of the modeled quarter domain, with the cutout representing the position of the building foundation, as usual. The crack for entry of soil gas and contaminant is in the corner of the foundation cutout. The bottom of the domain is at the top of the water table, through which soil gas flow cannot pass.

While not so easily visible given the scale of the figure, the pressure near the foundation crack region is very near the assumed house depressurization of -5 Pa. This is of course because the entrance to the crack was specified as a boundary condition at that value. But moving away from the crack, the pressure quickly approaches that at the ground surface, though the underside of the foundation slab is still very slightly depressurized relative to the ground surface. As must be the case, the flow streamlines are orthogonal to the isobars, as may also be seen from this figure. It should be emphasized that the streamlines are not conveying information regarding the flow velocities, but merely the path that is followed by the flow that passes a particular point. The streamlines converge to the point of entry of soil gas into the house, at the foundation crack. The source of the air entering the foundation is seen to be the ground surface. The most important path for providing the air that flows through the soil is that which offers the least resistance to flow, which would be that which originates directly adjacent to the foundation.

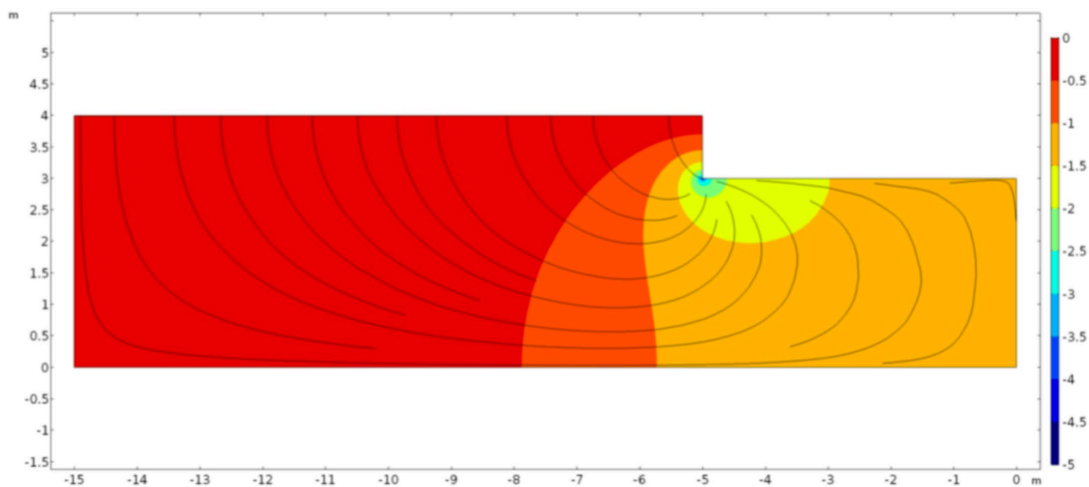


Figure 2.16. Pressure Field from Darcy's Law and Associated Airflow Streamlines.

Color scale indicates pressure relative to atmospheric, in Pa.

Figure 2.17 shows the contaminant concentration profile in the soil, corresponding to the soil gas flow pictured in Figure 2.16. The concentration values are normalized to the groundwater source concentration and are plotted as the logarithm of that normalized ratio. The portion of the profile immediately above the groundwater surface is seen to reflect that the contaminant concentration quickly falls by one to two orders of magnitude in a short vertical distance, reflecting the very significant resistance to diffusion in the capillary zone right above the top of the water table.

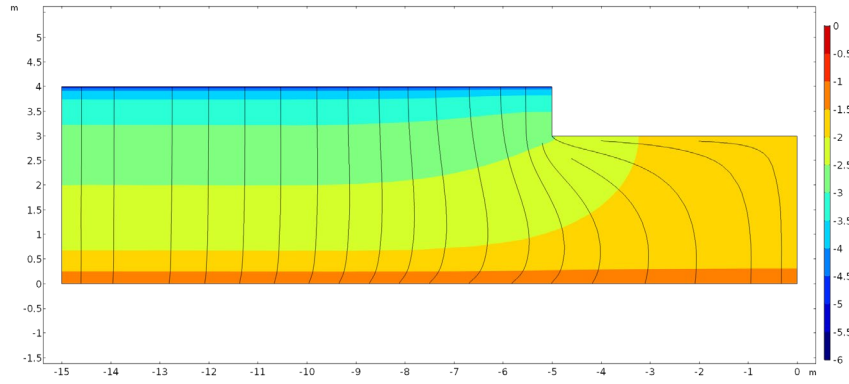


Figure 2.17. Contaminant Concentration in the Soil, Plotted as the Logarithm of Contaminant Concentration Normalized to Groundwater Concentration.

Also shown are the streamlines for advection-diffusion of the contaminant.

At a distance of a few meters from the foundation, what is observed in Figure 2.17 is the result of a simple process of diffusion from the groundwater source to the atmospheric sink. This figure also illustrates why it is generally difficult to use soil gas contaminant measurements taken outside the footprint of the structure to estimate the subslab concentration directly beneath the structure. Underneath the foundation slab, the contaminant concentration builds up as a result of the blocking effect of the building on the upward diffusion process. The flow paths of contaminant beneath the building show that they bend towards the edges of the building foundation. By analogy with streamlines, the flow paths for diffusion of the contaminant vapors are normal to the concentration isoquants. This behavior indicates that the influence of soil gas advection is not very significant in determining the flow paths of contaminant. The concentration of contaminant immediately adjacent to the entry crack is 3 orders of magnitude lower than the concentration at the groundwater vapor source.

The fact that immediately below the slab the soil gas flow streamlines are so similar to the paths shown for the contaminants might seem to suggest that the contaminant movement there is advectively determined. This is not the case, as may be seen by inspecting Figure 2.18, which shows actual airflow velocities. This figure shows that the actual influence of the building depressurization on moving soil gas is very small, except in the immediate vicinity of the foundation entry crack.

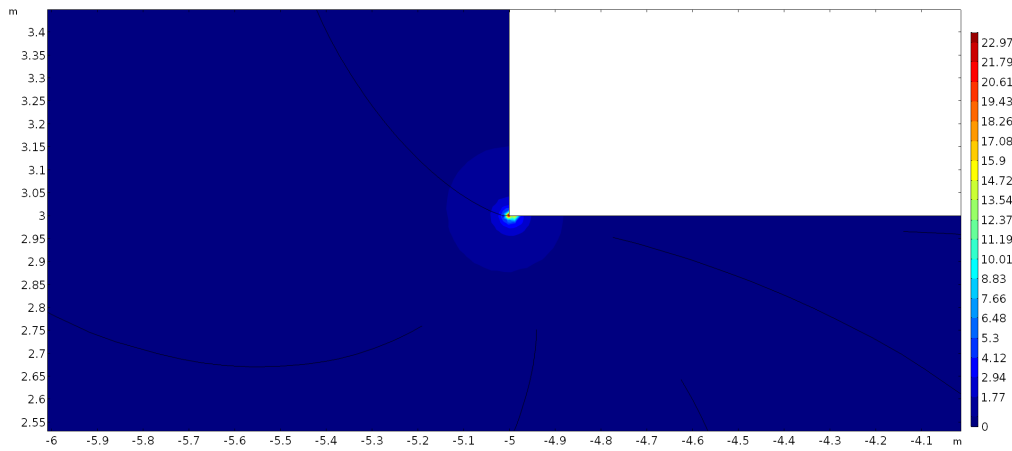


Figure 2.18. Airflow Velocity u_g [mm h⁻¹] Near the Foundation Crack.

The above conclusion is reinforced by Figure 2.19, which shows the magnitude of the horizontal component of contaminant diffusive flux as compared with the total flux at any point. The areas of green outside of the building footprint indicate a zero horizontal flux component, consistent with the upward diffusional movement of the contaminant in that area. The blue areas directly beneath the building slab have a value of -0.8 or greater, indicating that the movement of contaminant is from right to left and is almost entirely dominated by diffusion. It is only very near the entry crack that a small region (the yellow/red area) with a positive ratio is seen, indicating that there is significant movement of contaminant from left to right (towards the crack) and that it is somewhat influenced by advective flow.

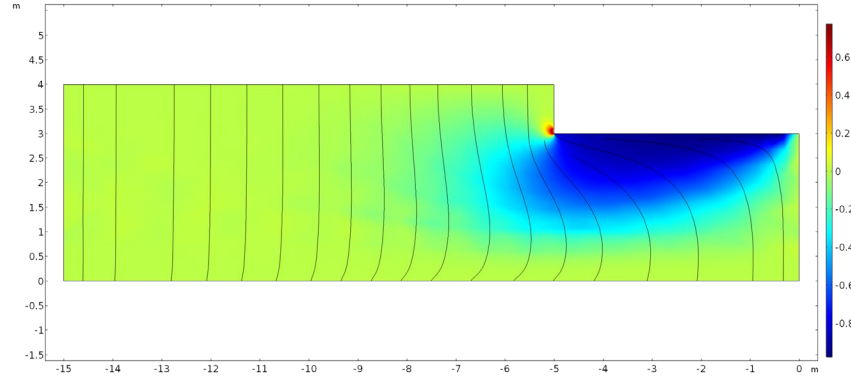


Figure 2.19. Horizontal (y-axis) diffusive Flux Component Normalized to the Magnitude of the Total Flux.

A value of 0 here indicates that there is no horizontal component of diffusion (it is purely upward). A value of +1 or -1 indicates that the horizontal component of contaminant transport is purely determined by diffusion (the sign indicates diffusional direction, with positive values indicating a flux to the right). For example, a value of -0.8 indicates that the 80% of the magnitude of the contaminant transport is due to horizontal (along the y-axis) diffusion, and occurs leftward.

The above results confirm what has been previously hypothesized about the nature of the vapor intrusion process. Diffusion dominates the process by which contaminant vapors travel from groundwater source to foundation. The influence of advection is only felt very near to the foundation breach, where the small degree of indoor depressurization can influence soil gas entry rate into the building. This example shows the power of numerical modeling to predict subtle details of the VI process that would otherwise not be apparent.

Post-processing may also be used for searching for “bugs” in the programming or inputs, and for evaluating where the mesh can be potentially improved. Numerical solution of the species transport equation sometimes leads to the solution oscillating around the “true” solution (seen as significant oscillatory differences in concentration between nearby elements), especially if the mesh size in a particular region is too large. This problem can be identified by examining the cell Péclet number, which characterizes the relative magnitudes of advection/diffusion in any element or “cell”.

$$Pe_{cell} = \frac{\text{advective transport in cell}}{\text{diffusive transport in cell}} = \frac{u_{gas} h}{2D_{eff}} \quad (2.37)$$

here u_g [m s^{-1}] is the soil-gas airflow velocity, h [m] is the mesh size of the element or cell, and D_{eff} [$\text{m}^2 \text{s}^{-1}$] is the effective diffusivity within the cell. If $Pe_{cell} > 1$ there is a risk that this oscillating behavior will manifest. Small exceedances, e.g., $Pe_{cell} < 25$, are usually mitigated by numerical stabilization schemes that are integrated into COMSOL, as well as into many other FEM packages. For larger values of Pe_{cell} further mesh refinement may be required.

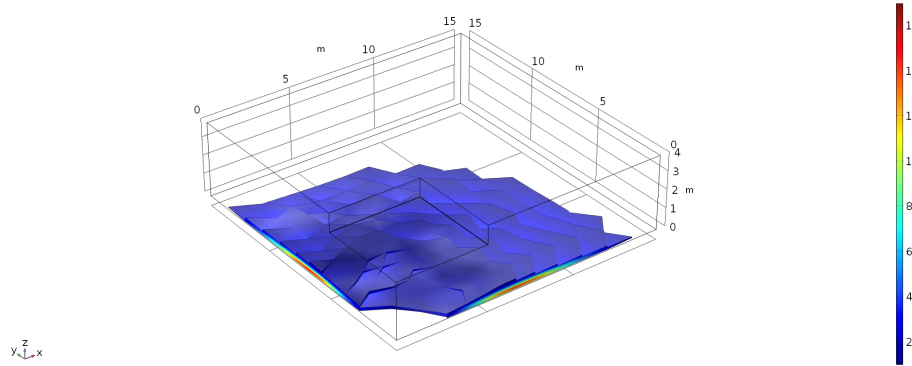


Figure 2.20. Volume Plot of the Same Model System as in Figure 2.17, Showing Where Cell Péclet Numbers Exceed 1.

Figure 2.20 shows a plot of Pe_{cell} as a volume plot. It excludes all values of $Pe_{cell} < 1$. Only the region close to the groundwater exceeds the above stability criterion, which is attributable to the very small D_{eff} in that part of the domain. The exceedance of the criterion is so small, such that the built-in numerical stabilization scheme is able to compensate, as confirmed by examining the region near the groundwater source in Figure 2.17 (no oscillations in concentration are visible).

2.6 THE USE OF STEADY STATE NUMERICAL MODELS IN SUPPORT OF OTHER MODELING AND VI INVESTIGATION

It has already been noted how the concepts on which numerical models can be traced back to the Johnson-Ettinger model [42] and its forerunners in the radon intrusion field. That work led to the development of spreadsheet implementations of that model [7], whose performance has been checked by comparison with the 3D numerical models such as that just described in the preceding sections [43]. There are various other VI models used in many European countries, which have also been reviewed [68]. Most are based upon the same basic physical concepts. However, a main impediment to using any models in VI investigations has been the difficulty in validating their predictions. This needs to always be kept in mind in using the techniques described above. As tempting as it might be to believe that all of the “relevant” parameters and processes have been included, this is always a dangerous assumption.

One thing that numerical modeling has enabled is the development of simpler 2D analytical models of the VI process. These analytical models are never as comprehensive as the full 3D numerical models, but they have the advantage of lending themselves to capturing many of the aspects of 3D models but allowing for rendering of the better approximations to the real situation than is possible with 1D models, but without the effort of implementing the full numerical model. One of the first efforts in that direction was that by Yao et al. [69].

This has been followed by other efforts in this direction by Yao and Verginelli [70-72]. These analytical approaches have been implemented in simple spreadsheets, available at *pvttools.net*. Again, it was the ability to check the analytical solutions against the full 3D numerical solutions that gave impetus to, and confidence in, the approximations that are used in these efforts.

2.7 EXTENSION TO MODELING OF TRANSIENT VI PHENOMENA

A main driver for this project has been the need to explain the wildly time-varying indoor air contaminant concentrations seen at several important VI study sites. This might suggest immediately moving to the full implementation of the VI model with transient terms. There is, however, significant value in exploring the steady state models presented above, prior to exploring the computationally much more demanding transient models. The steady state models can be run at the conditions defining the bounds of the transient analyses, and point out the input parameters that define the sensitivity of the solutions. The steady state solutions can be used to assure that the transient models are converging to reasonable limiting cases.

Some of the required equations are but little modified from what was used in the steady state analysis. The major change is, of course, the inclusion of a time dependent term. The required changes are now outlined.

Calculation of Indoor Air Concentration

The indoor air contaminant concentration is still the main dependent variable of interest. The time-dependent governing equation for c_{in} is a simple expression for conservation of contaminant mass in a well-mixed volume. The time dependent inventory of contaminant (the left-hand side of the equation) depends upon the difference between contaminant entry rate and its being flushed out by air exchange:

$$V \frac{dc_{in}}{dt} = n_{ck} - V A_e c_{in} \quad (2.38)$$

where, as earlier, c_{in} [mol m⁻³] is the indoor contaminant concentration n_{ck} [mol s⁻¹] is the contaminant entry rate into the building via the foundation crack, A_e is the air exchange rate and V is the volume of section of the building that is impacted, i.e., the structure's basement, in the model developed here. Note that equation (2.38) reduces to equation (2.1) when the time derivative is set to zero (i.e., the steady state condition). In the general transient case, both n_{ck} and A_e can be time dependent, and either or both can be important in driving the time dependence of c_{in} . This makes the solution of this ordinary differential equation difficult, because all terms can have complicated time dependencies. As in the steady state case, the value of n_{ck} must be determined from equation (2.6) in which j_{ck} is now time-dependent. As before, the value of j_{ck} at any instant of time is governed by equation (2.10), subject to the same limiting cases as shown in equations (2.11) and (2.12).

Modeling Airflow Under Transient Conditions

The advective motion of soil gas is still required in order to understand the transport of contaminant. As before, the main interest is in the motion of the gas phase, and the motion of liquid water in the vadose zone is neglected (unless the interest is in the movement of precipitation through the vadose zone, not considered further here). Thus, the unsteady state form of the continuity equation, combined with Darcy's Law (2.20) can be written as:

$$\frac{\partial}{\partial t}(\rho\theta) + \nabla \cdot \rho \left(-\frac{k}{\mu} \nabla p \right) = 0 \quad (2.39)$$

in which ρ is the density of air, θ is the porosity available for soil gas flow, k is the permeability, and μ is the viscosity of air. Again, the soil gas is taken as essentially incompressible, so ρ is constant. This reduces (2.39) to essentially the same as (2.22), and the same process as before can be used to derive the desired velocity field. What does change is the fact that the pressure boundary condition at the foundation crack entrance may be time dependent, which drives the time dependence of the velocity field.

Contaminant Transport in the Vadose Zone Under Transient Conditions

Use is now made of the result shown in (2.35), just allowing for the unsteady state accumulation of contaminant in the three phases in which it can exist- vapor, dissolved in water, and adsorbed to soil.

$$R \frac{\partial c_w}{\partial t} = \nabla \cdot [D_{eff} \nabla c_w] - K_H \mathbf{v} \cdot \nabla c_w \quad (2.40)$$

In which the definition of R is as before:

$$R = (\theta_w + \theta_g K_H + K_H K_p \rho_b) \quad (2.41)$$

and

$$D_{eff} = (D_w \frac{\theta_w^{10/3}}{\theta_t^2} + D_g \frac{\theta_g^{10/3}}{\theta_t^2} K_H) \quad (2.42)$$

Again, the value of c_w is now time dependent, and with that, all of the other contaminant concentrations as well. To the extent that this is the case, processes related to adsorption/desorption from both the solid and water phases must now be considered. It is generally assumed here that the equilibrations between phases are so rapid as to not require additional consideration of rate constants for these processes. The following sections of this report give examples of the use of the numerical models described above.

3.0 EXAMPLES OF THE USE OF NUMERICAL MODELING TO ANALYZE TRANSIENTS IN VAPOR INTRUSION

It has been recently concluded that a preferential pathway plays a key role in the case of the significant contaminant concentration transients observed at the ASU vapor intrusion study house outside of Hill AFB [23,24]. The question that numerical modeling can help address is what factors are necessary for creation of the observed very large transients. In other words, numerical modeling can indicate what may be generalized from the observations at this one particular site.

The nature and effects of what might be believed to constitute a “preferential pathway” can vary greatly from site-to-site. Generalizing their impacts can therefore be difficult. It will be shown that it is not necessarily the case that the mere existence of a conduit containing contaminant vapor can lead to the observed impacts. In fact, the EPA experimental house in Indianapolis was also affected by a preferential pathway, but the role and influence of that pathway was very different from that at the ASU house. It is also the case that a preferential pathway is not necessary for significant transients to be observed at a VI site; the results from Naval Air Station North Island establish this.

Preferential Pathways

A preferential pathway is typically thought of as involving some sort of conduit (or flow path of low resistance) that can transport contaminant vapors into a building at a rate greater than the normal slower vapor transport through soils, as characterized the example VI model of the previous section. At the ASU house, this took the form of a land drain located underneath the building’s foundation slab. This conduit was presumably installed during house construction in order to drain excess water from the sub-slab region. This land drain was connected to a nearby sewer located some meters in front of the house. The entrance of the drain was located in a gravel sub-base layer under the house foundation. Installation of this sort of gravel sub-base is quite common in foundation construction- the concrete slab is often poured directly atop this gravel layer.

The sewer pipe to which the land drain connected was buried deep enough to be partially submerged in the TCE contaminated groundwater. It is likely that the contaminated groundwater infiltrated into the sewer, filling the vapor space of the normally dry land drain with TCE-contaminated vapor. When the ASU research team discovered the land drain after many months of measurements had been performed at the house, it was excavated and fitted with a valve, allowing it to be isolated from communicating with the gravel sub-base [23]. It should be noted that the preferential pathway in this instance did not actually enter the structure- it dead-ended in the gravel sub-base. There was, however, a foundation breach that permitted vapor communication between the interior of the house and the gravel sub-base.

At the EPA duplex, an ordinary sanitary sewer acted as a preferential pathway for entry of contaminants into the structure [22]. While this situation had some similarity to that at the ASU house, the nature of this preferential pathway was quite different. A tracer gas test demonstrated that contaminant vapors were transported from the sewer into the duplex [22]. This is similar to what was observed at a site in Somerville, Massachusetts, where PCE entered into a bathroom through broken plumbing fixtures [21]. At the EPA duplex it was demonstrated that contaminated groundwater infiltrated into the sewer a few blocks away from the duplex, from an area where a dry-cleaners had previously been located. This type of distribution of contaminant vapor via a sewer network had been previously reported in Denmark [73].

It is likely that the sewer pipe at the duplex also leaked contaminant vapors near to, but outside of the foundation of the house. This added an aspect similar to that existing at the ASU house, in which the land drain never actually connected directly to anything within the structure. It is apparent that all of these different possible entry pathways are substantially different than the traditionally assumed groundwater-via-soil-to indoor pathway, which was the subject of the example calculations described in section 2.

Figure 3.1 shows a visual summary of the different possible entry processes involving preferential pathways. It is immediately apparent that these would not be modeled using the equations developed in section 2. Fortunately, because of how the investigation at the ASU site evolved, it was possible to use the results from that site to examine both the “traditional” pathway and the preferential pathway at the same site. The influence of the preferential pathway at the ASU house could be turned on and off at will (using a valve on the land drain). This permitted examining how the equations governing VI at the site were influenced by the existence of the preferential pathway.

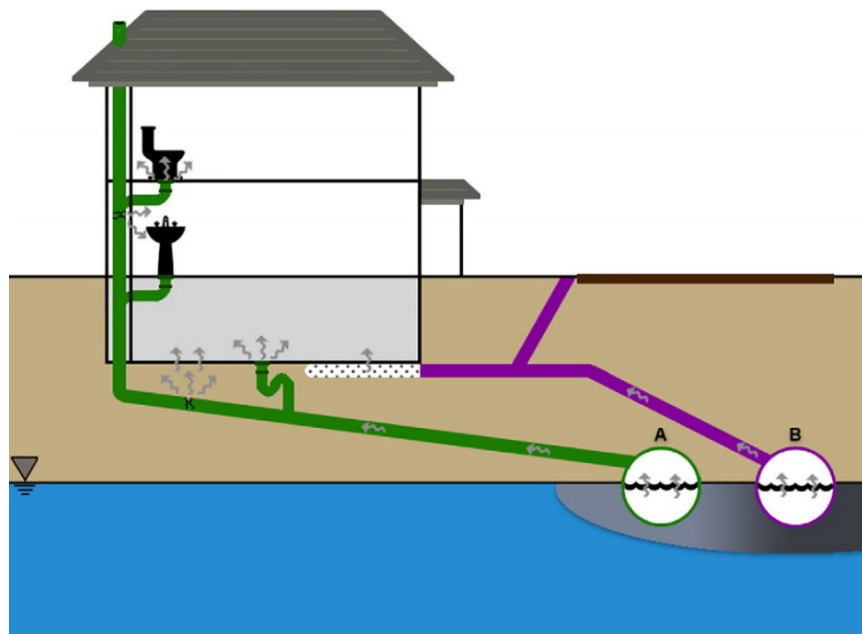


Figure 3.1. Visual Summary of Some of the Different Ways that Contaminant Can Be Transported Into a VI-impacted Building Via Preferential Pathways.

Figure from McHugh et al. [22].

3.1 OBSERVED VI BEHAVIOR AT THE ASU/HILL AFB HOUSE

This site was remarkably well characterized and thoroughly studied. We are grateful to the investigators from ASU for sharing with us the raw data from this site. The investigators monitored various metrics relevant to VI, such as building pressurization, air exchange rate, indoor and outdoor temperature, and other metrological variables, while simultaneously monitoring the indoor air contaminant concentration. Additionally, soil-gas and groundwater contaminant concentrations beneath and around the house were monitored. The specific sampling locations, as well as a photo of the house, are shown in Figure 3.2. The details of the experimental setup, and measured metrics, are detailed by Holton et al. [24].

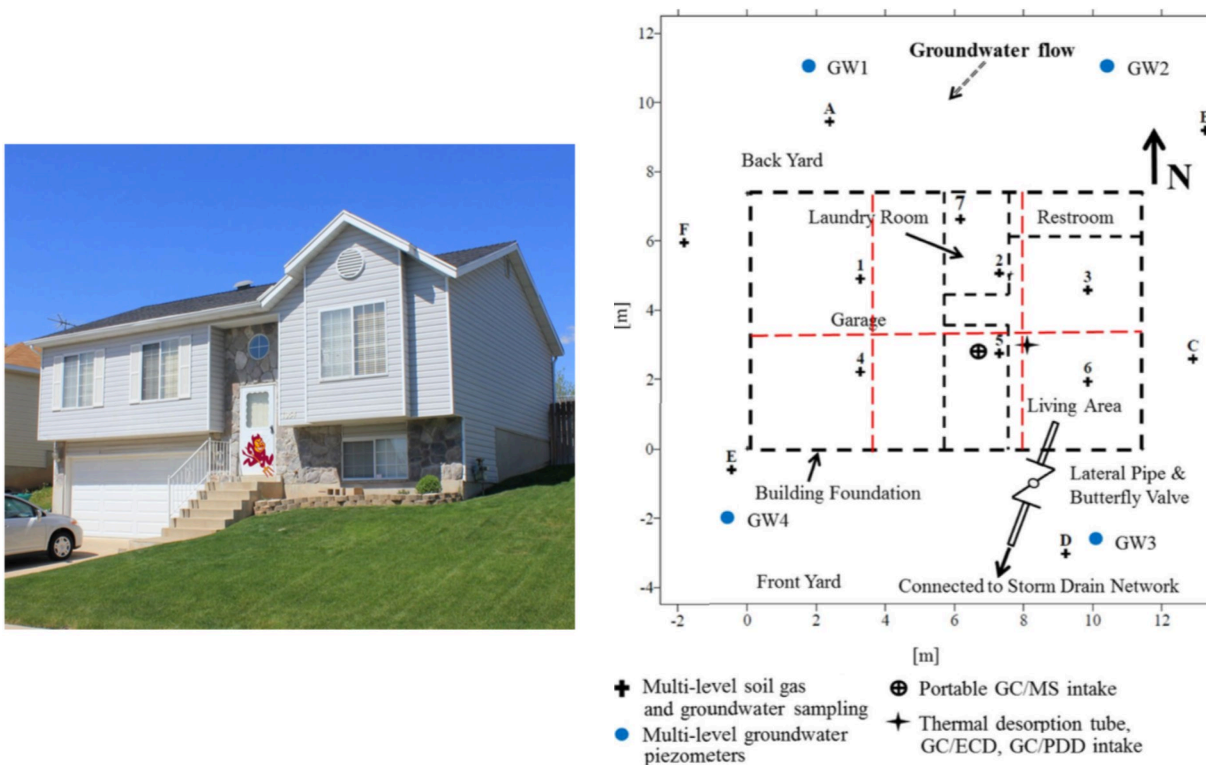


Figure 3.2. The “ASU House” VI Site Outside of Hill AFB in Layton, Utah.

Left hand panel shows a picture of the ASU house from Holton et al. [24]. The right hand panel shows a floor plan of the lower level of the house. Locations of all sampling ports and of the land drain (preferential pathway) marked. Figure from Guo et al. [23], in which the red dashed lines indicate subareas for making high-resolution emissions estimates in that field study.

This site was impacted by TCE. It was studied for roughly 1.5 years before testing using the controlled pressure method (CPM) was begun. During the time before the CPM tests, it was established that indoor air TCE concentrations fluctuated significantly at the site - roughly an order of magnitude on a weekly basis, and up to three or more orders of magnitude over different seasons. Once the house was depressurized using the CPM regime, indoor contaminant concentration increased to the highest concentration levels previously recorded. This was viewed as providing a validation of the CPM testing strategy [29]. The results obtained during the CPM testing period are shown in Figure 3.3.

It was, however, observed during the CPM testing period that the house and a nearby sewer were seemingly communicating with each other. This was demonstrated when a plastic tarp covering a nearby sewer manhole, reacted to the opening and closing of a door of the house. Further investigation led to the discovery of the land drain preferential pathway at the site. The location of the land drain relative to the house floor plan is shown in Figure 3.2. The land drain was determined to exit into a gravel sub-layer beneath the foundation slab, quite near a visible cm-scale opening between the foundation slab and foundation wall. The land drain was subsequently excavated and fitted with a butterfly valve [23] to control its influence. The land drain was closed towards the later part of the CPM study, which led to a significant decrease in indoor contaminant concentration. This effect can be seen in Figure 3.3, which shows the measured indoor TCE concentration for the entire study period. Note that the temporal variability in indoor contaminant concentration decreased significantly after the closing of the land drain.

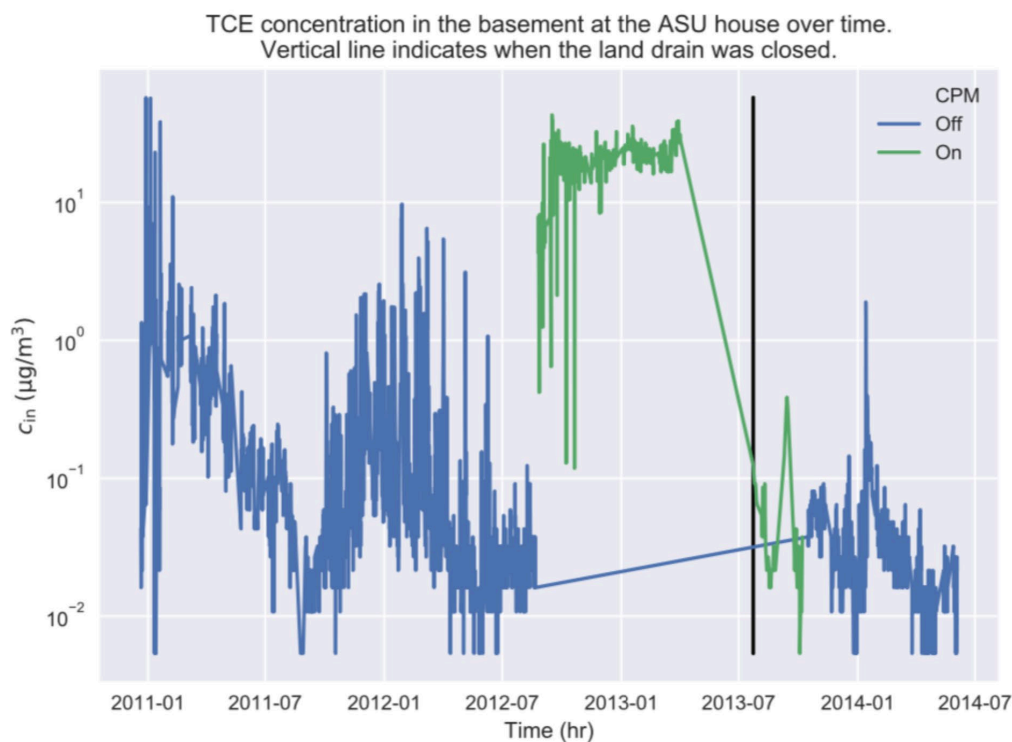


Figure 3.3. The temporal variability of Indoor air TCE Concentrations Recorded at the ASU House.

Measurements were taken in the basement. The periods during which CPM testing was performed are indicated.

Figure 3.4 shows the same data as in Figure 3.3, in the form of a boxplot. The boxes represent the interquartile range (IQR) of the distribution - the middle line of each box is the median value, and the top and bottom of the box represent the 75th and 25th percentile values, respectively. The whiskers are the extent of what is considered the reliable dataset, while isolated “outlier” points are indicated by the dots (these are defined as data lying 1.5 times outside the IQR).

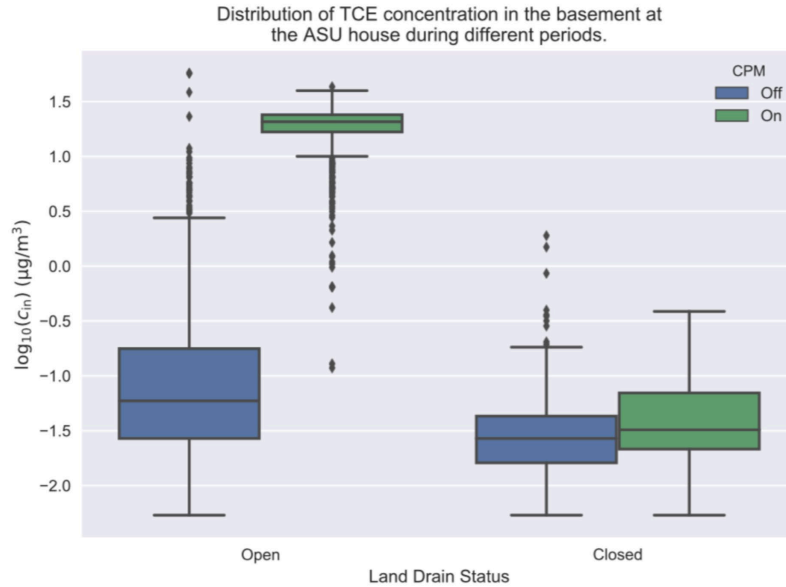


Figure 3.4. Boxplot Showing Measured TCE Concentrations (As Logarithmic Values).

It is commonly assumed as a basis for the controlled pressure method that the degree of depressurization of the building relative to ambient determines contaminant entry into VI impacted building. This presumes an advectively determined entry rate into the structure, but there is typically no a-priori reason to believe that this is the case. If the entry rate into a structure through the foundation breaches were instead diffusion rate controlled, the small degree of depressurization employed during the CPM would have negligible effect on the diffusivity of contaminant through the crack, and the influence of CPM on indoor air contaminant concentration would be negligible. This point may be considered by examining the data from the ASU house.

Figure 3.5 considers the relationship between the indoor air concentration and the extent of building pressurization or depressurization, for the periods when the preferential pathway was either open or closed. Creating this figure involved cross-plotting the measured indoor air TCE concentrations with the corresponding measured indoor/outdoor pressure differences. The results clearly show the dramatic decrease in sensitivity of the indoor contaminant concentration to the extent of building depressurization following the closing of the preferential pathway. The use of a linear fit to the data is clearly not appropriate for the data set from when the land drain was open, but the actual relationship between these variables will be further explored when the numerical VI models are applied to describing this situation.

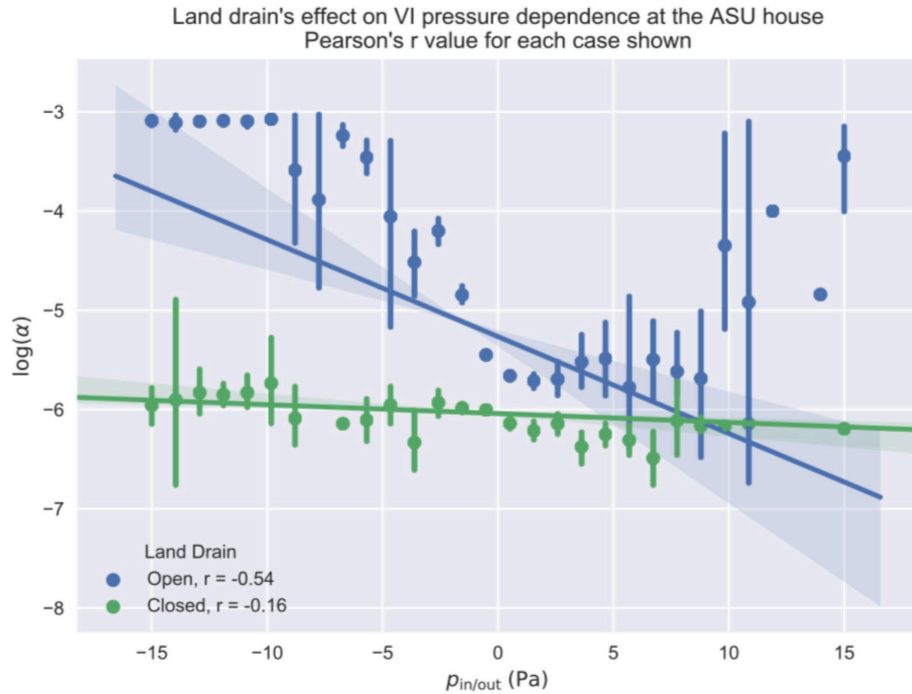


Figure 3.5. The Effect of Indoor/Outdoor Pressure Difference on Indoor Air TCE Concentration in the ASU House.

Here the indoor air concentration has been normalized to the groundwater source concentration, i.e. it is represented as an attenuation factor. Data have been placed in evenly spaced (but not sized) pressure “bins”. The bars indicate the 95% confidence intervals within each pressure bin.

The fundamental shift in the relationship between building pressurization and indoor air contaminant concentration indicates that there is a significant role of the preferential pathway when it is open. Examining the reasons for this behavior was one of the primary objectives of this study, since this helps address the question of the very large temporal variability in indoor air concentrations while the pathway is open. Numerical modeling will offer a very clear explanation of this phenomenon.

3.2 OBSERVED VI BEHAVIOR AT THE EPA STUDY HOUSE

The EPA duplex was also the subject of a highly detailed VI study for an extended period of time. Figure 3.6 shows a photo of the EPA study site. Indoor air contaminant concentrations of TCE, PCE, chloroform, and radon were all measured on different floors of each side of the duplex, as well as in different locations and depths in the subsurface and groundwater. The sampling locations, as well as a floor plan of the duplex can be seen in Figure 3.6. Pressure differences between different locations were also measured. Metrological data were collected throughout the study period, which lasted for around 2.5 years, and included indoor and outdoor temperatures, wind speed and direction, precipitation, and snow coverage [74]. The data from this site are publicly available online [75].

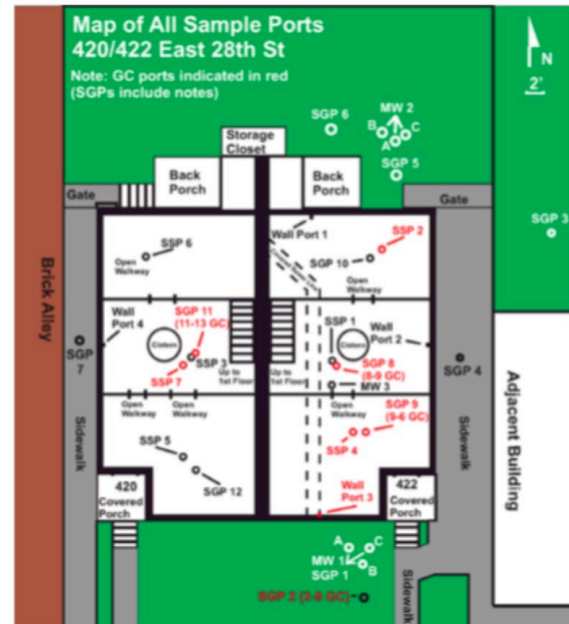


Figure 3.6. The EPA Duplex VI Study Site in Indianapolis, Indiana.

As with the ASU site, this site was likewise characterized by significant temporal variability in measured indoor air contaminant concentrations. Typical data, for TCE, are shown in Figure 3.7. While the variability in contaminant concentrations was not as significant as was observed at the ASU house, it was substantial nonetheless. Once again, seeking an understanding the observed variability was a major focus of this study. At this site, the effects of a subslab depressurization (SSD) mitigation system was also studied, but here, only data taken prior to the implementation of the SSD system are the focus. Also, only one side of the duplex house was heated, and only data from that side are considered.

As in the case of the ASU house, it was determined during the studies on this site that there existed a sewer preferential pathway [22]. This preferential pathway seemingly played a very different role than the one that impacted the ASU house. Communication between this preferential pathway and the indoor environment does not seem to have been as strong which may have been due to the poor condition of the sewer pipe, which might have leaked along its path (this will be discussed below).

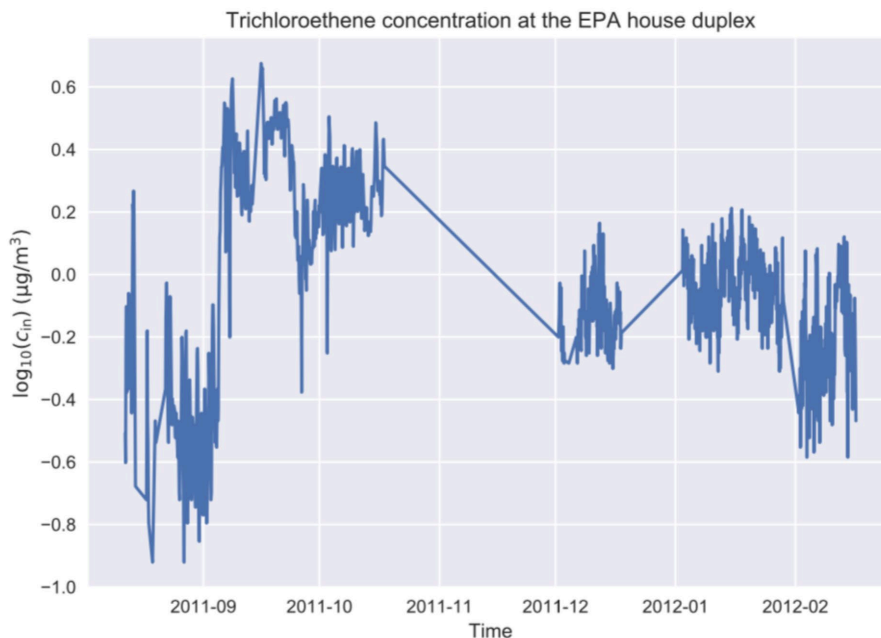


Figure 3.7. Sample Indoor Air TCE Concentrations at the EPA VI Study Site.

The data in Figure 3.7 illustrate an almost two order of magnitude variation in measured concentrations during this sampling period. Because at this site several contaminants were simultaneously tracked, there is additional information on the temporal variation of VI contaminants of concern. Figure 3.8 shows a boxplot of TCE as well as PCE and chloroform. These data suggest that the variation in TCE concentration was somewhat greater than that observed for the other contaminants.

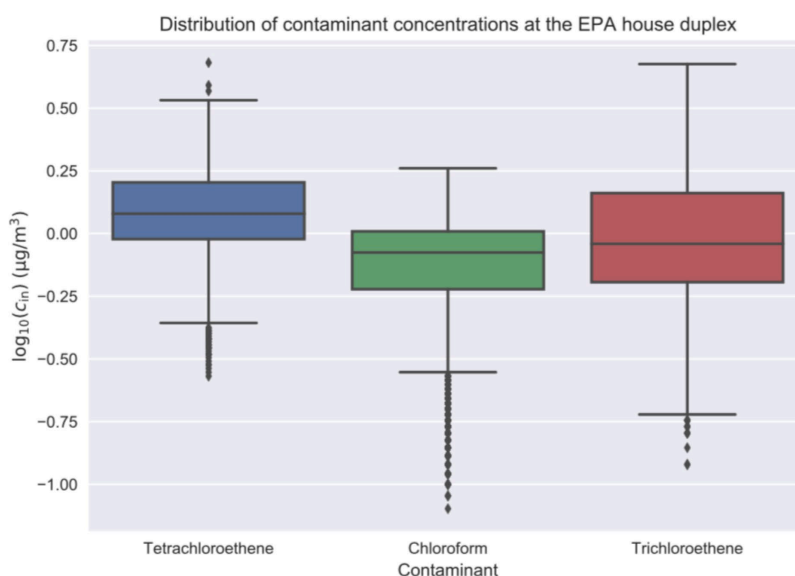


Figure 3.8. Boxplot Showing the Concentration Variability of TCE, PCE and Chloroform at the EPA VI Study Site in Indianapolis, IN.

Figure 3.9 shows how the indoor air contaminant concentrations for TCE, PCE and chloroform were related to the indoor/outdoor pressure difference. There is a very clear trend visible in all three data sets- the greater the indoor depressurization, the higher the observed concentrations. This is strongly suggestive of there being a role for advective entry of all of the contaminants into the structure.

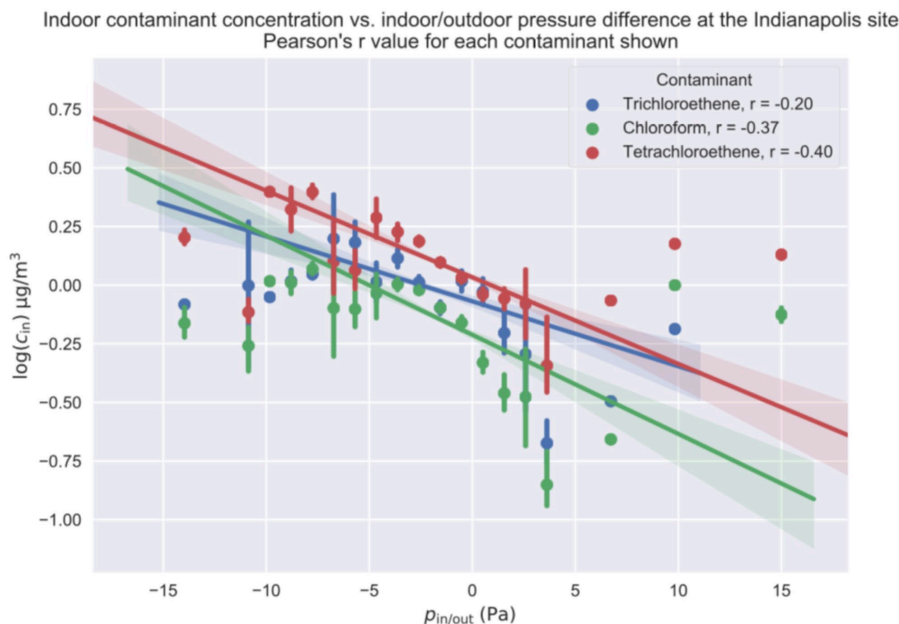


Figure 3.9. The Relationship Between Indoor Air Contaminant Concentrations and the Indoor/Outdoor Pressure Difference at the EPA VI Study Site.

It is, however, not nearly as clear how much the sewer preferential pathway contributed to indoor air contaminant concentrations at this site, since its effect was never isolated as it was at the ASU house. There was a sewer pipe that led into the building, and the sewer was observed to contain contaminant vapors [22]. The evidence from this site suggests that the sewer line might actually have delivered contaminant vapor to the soil immediately adjacent to the structure, via a break in the sewer line. Breaks in sewer lines are not at all uncommon, and sewer lines, once placed, are rarely maintained. This possibility was considered in modeling this site.

3.3 ADDING CONSIDERATION OF A PREFERENTIAL PATHWAY TO A VI MODEL

The Physical Layout

In this section, the process of enriching the model to include consideration of a preferential pathway is illustrated by focusing first on the ASU study site. The addition of a preferential pathway to the basic numerical model of vapor intrusion was an essential element in explaining the observed wide temporal variability in indoor air contaminant concentrations at that site. This required adding to the earlier presented model a gravel sub-base layer underneath the foundation slab and a preferential pathway conduit. No attempt was made to model exactly the layout of the ASU site, but the key details were chosen to be of reasonably similar dimensions.

It was assumed that the house had a gravel sub-base layer that was 30 cm thick and that it extended just beyond the edges of the foundation slab. It had been established that there was such a gravel sub-base at that site, and while its exact thickness was not known, it was assumed that it was of typical thickness in US residential construction. This gravel sub-base thus formed a uniform layer immediately beneath the foundation slab, and it sat atop homogenous sandy clay, that characterized the rest of the vadose zone. This choice of soil was consistent with the assumptions in other modeling work on the site by Guo [76]. The gravel sub-base is normally dry, but for consistency in modeling the soil and gravel layers, van Genuchten parameters for the gravel are also considered, even though they do not imply significant moisture content. (See Table B.1).

The preferential pathway (the land drain, in this case) was modeled as a 10 cm diameter pipe that exits at the interface between the soil and gravel sub-base layer. It was assumed to terminate near the foundation crack, as was actually observed to be the case at the site [23]. Figure 3.10 illustrates the assumed scenario.

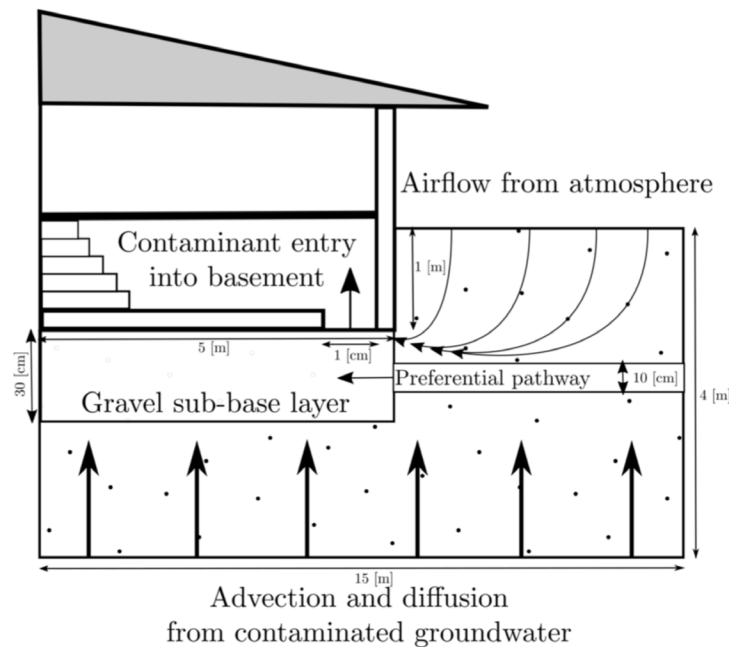


Figure 3.10. The Modeled Preferential Pathway VI Scenario.

Meshing

Since contaminant vapor transport within the preferential pathway itself was not of interest, only the exit of the pipe was modeled. The pipe exit was modeled as a 10 cm diameter circle representing the boundary between pipe and gravel. Otherwise, the same considerations as before still apply in developing a mesh, except that there are now two separate soil layers (actually a gravel and a soil layer) to consider.

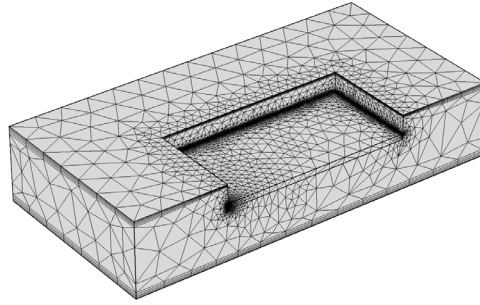


Figure 3.11. Meshed Geometry of the Preferential Pathway Model, Including the Gravel Sub-base Layer and the Preferential Pathway Exit (Near the Left Hand Foundation Crack).

Addition of the preferential pathway pipe also removes one of the earlier planes of symmetry (since the pipe enters from only one side of the structure). Thus, only one plane of symmetry now exists instead of two, and it is necessary to model half of the domain model geometry instead of just a quarter as was done before. The meshing of the new situation is shown in Figure 3.11. On the scale of Figure 3.11, the area around the exit of the preferential pathway is barely visible as a darker cluster or mesh nodes in the lower left side of the cutout representing the foundation. A boundary layer mesh has been generated on the circular preferential pathway exit plane. Otherwise, the initial mesh is quite similar to that generated earlier. The meshing in this case will also be subject to subsequent adaptive mesh refinement.

The New Boundary Conditions

In the revised model that includes the preferential pathway, the governing equations introduced in Section 2.5.2 of this report (and summarized in Figure 2.10) are still all relevant. It is, however, necessary to supply new boundary conditions - one related to how the airflow is impacted by the presence of the preferential pathway, and the other for the fact that the preferential pathway represents a contaminant source. The addition of the gravel layer does not change the structure of the equations, since it is treated like any other soil layer. The main difference from the basic example is that there is a change in the properties of the soil, in the transition from the surrounding soil to the gravel sub-base. This does not result in addition of any new equations for airflow or contaminant transport in the soil- only the transport properties change at the interface because of the different van Genuchten parameters for the two layers.

Since the preferential pathway is in this case assumed to be an open pipe that simply dead-ends in the gravel layer, it offers no obstruction to flow. Its other end is attached to a sewer that communicates freely with the atmosphere. Consequently, the assumption was made that the end of the pipe in the gravel sub-layer would be at the external ambient pressure. Consequently, in this case, the new boundary conditions for application to Darcy's Law are:

Ground Surface	$p = 0$
Foundation crack entrance	$p = p_{in}$ (e.g. -5 Pa)
All remaining boundaries	No flux (i.e., $v = 0$ normal to surface)
At the pipe exit	$p = 0$

Thus, the only addition to the boundary conditions for Darcy's Law is the last of these equations. Rather than specifying that the value of the indoor air pressure (felt at the crack entrance) is always -5 Pa as in the previous example, it is here indicated that this value will be parameterized in the analysis that follows.

It is assumed that the air in the preferential pathway pipe is contaminated with TCE at a vapor concentration c_g , which is the same value that is in equilibrium with the groundwater source. This assumption is based on observed contaminant concentrations in the sewer near the ASU house [76], i.e., contaminant vapor concentrations in the nearby sewer were of similar magnitude as those at the contaminated groundwater source. Thus the boundary conditions for the contaminant advection-diffusion equation are:

At the ground surface $c_g = 0$, or equivalently, $c_w = 0$

At the groundwater surface $c_w = c_{w, \text{source}}$

At the foundation crack, flux $= -j_{ck}$

All other solid boundaries – No flow.

At the preferential pathway exit, $c_g = c_{gw}KH$

Again, the only new boundary condition is the last one, showing the pipe to be a source of contaminant. Note that sorption to the soil is again neglected because this is a steady state analysis.

3.4 MODELING RESULTS FOR A PREFERENTIAL PATHWAY CASE

The model presented above is a steady state model, but as will be demonstrated, its results offer important insights into what drives the very large fluctuations in indoor air contaminant concentration observed at the ASU study site. The results obtained by assuming different values of the indoor air pressure are illustrated in Figure 3.12. The indoor air exchange rate A_e was assumed to be a constant 0.5 hr^{-1} , and $p_{in/out}$ was varied from -5 to 5 Pa (where as before negative values indicated the “usual” situation of depressurization of the structure). The displayed c_{in} values calculated from the model were normalized by the assumed vapor concentration in equilibrium with groundwater c_{gw} , and thus given in Figure 3.12 as the attenuation from groundwater α_{gw} .

As noted above, while the intent was not to exactly model all details of the ASU study house. It became apparent early in the modeling process that it would be difficult to implement a full detailed model of this or any of the other sites, because no matter how much detail we built in, the available input parameters (i.e., field measurements) would not support those details (that is, the model can outstrip the availability of the actual site data). For example, at the ASU site, it was apparent that we could approximate the relative locations and dimensions of the preferential pathway and entry crack, but we would not be able to get very precise information on these. So rather than try to capture all of the details, we took the approach of modeling a site that was very close to the ASU site, but not claiming it to be an exact replica. The model nevertheless captured key details such as house footprint size, crack entry size, existence of a gravel sub-base, and the “land drain”. We then exercised the model with this site representation, and the model was seen to successfully predict the observed trends in α_{gw} with $p_{in/out}$ (the blue line and blue data points).

The model does, however, somewhat under-predict α_{gw} when the house is over-pressurized (positive values of p_{in}), but the predicted and measured values of contaminant concentration are very low under those conditions (note the use of a log scale in Figure 3.12). The more critical range of contaminant concentration is the higher range seen when the house is depressurized. Most significantly, the model captures that for even a small increase in indoor depressurization (0 to -5 Pa) a very large increase in the attenuation from groundwater, α_{gw} , (two orders of magnitude) can occur, noting that an increase in this value indicates an increase in predicted indoor air contaminant concentration.

The results of Figure 3.12 showed that the model captured the key observations of the transients in the field, and did so to better than an order of magnitude in the key range of contaminant concentration concern. But in no case would we have been comfortable trying to claim that we were modeling observed indoor air concentrations to within any particular percentage. For one thing, the actual field measurements showed that there were different values in different parts of the house. To try to reconstruct any particular value at any point would have required layering a separate indoor air mixing model on the vapor intrusion model itself. In addition, an analysis presented in section 3.6 below showed the key role that natural fluctuations in air exchange rate would cause, and measurements of air exchange rates were not made for the entirety of the data set. Hence, it would be unrealistic to try to define a metric for modeling success that is based upon a simple comparison with any one measured indoor air concentration.

The above suggests use an unusual metric for modeling “success”, using the degree of predicted variability in measured indoor air contaminant concentration results vs. what was observed as a function of key measured parameters, such as indoor-outdoor pressure difference. This really goes to the heart of what the project set out to do- to use modeling to explain why field investigators could see such wild swings.

Thus Figure 3.12 shows one of the key results of the modeling work – the very large fluctuations in observed indoor air contaminant concentration can actually be driven by very modest changes in indoor air pressure. The modeling work allowed further examination of why this was the case here, but might not be in other scenarios.

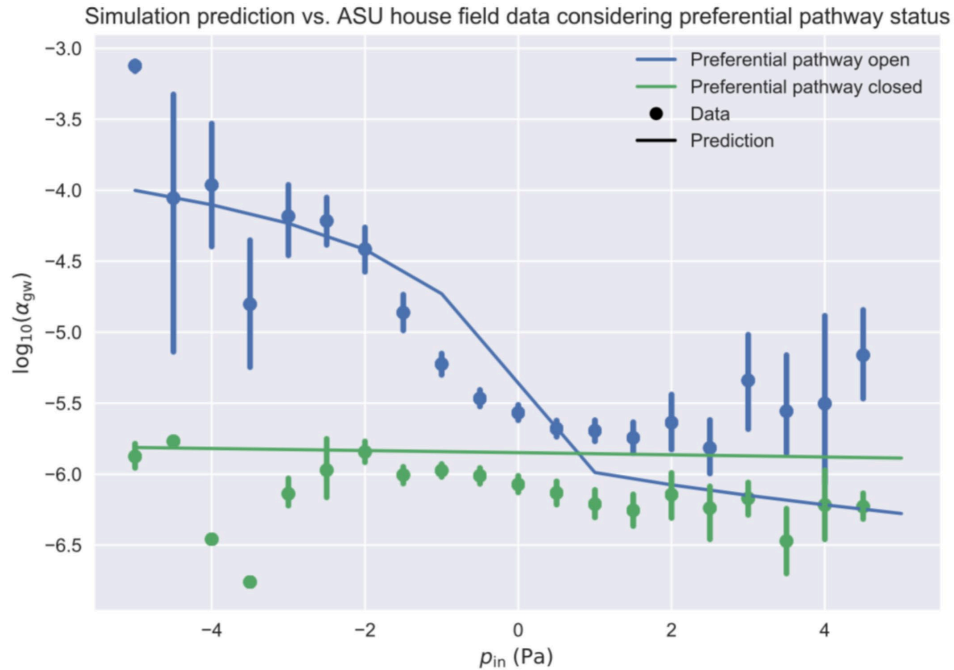


Figure 3.12. Predicted Indoor Air Contaminant Concentrations (shown as groundwater attenuation values) – solid lines. Actual field data from the ASU study site are shown as individual points. The blue line and points represent predictions and data for the situation prior to the closing of the preferential pathway. The green line and points represent predictions and data for the period following the closing of the preferential pathway. Here the data were placed in 20 equally spaced pressure “bins”. The “bins” near zero pressure contain many more data than those at the extremes of pressure. The data points represent the mean value of data at a given pressure, and the error bars represent the 95% confidence intervals for the data at that pressure.

In order to better understand the above results, a second calculation was performed for a case in which the preferential pathway is absent, but when there still exists a permeable gravel subslab region. This corresponds to the case in which the land drain preferential pathway was closed off. These results are shown as the green line and data points in Figure 3.12. The predictions are again in agreement with what was observed at the ASU study site, i.e. that there was a much more modest variation in indoor air concentration, irrespective of pressure, when the preferential pathway was cut off. The indoor air contaminant concentrations were roughly two orders of magnitude lower when the indoor air pressure was -5 Pa.

The modeling results thus corroborate the significant contribution that this kind of preferential pathway can have at a VI site, and are fully in accord with the conclusions drawn by the investigators at this site. The power of numerical modeling goes beyond this corroboration, however. This is because it permits variation of individual factors that cannot be controlled at the actual site. It is possible to separate out the effects of the preferential pathway as a source of contaminant vapor from its role as a source of air to the subslab. It also makes possible the examination of the role of a gravel sub-layer.

The preferential pathway acts not only as a source of contaminant vapor, but also as a source of air to the subslab. Insofar as the significant effect of pressure on predicted results strongly implies an important role of advective entry of contaminant into the structure, this raises a question regarding whether the effect of the preferential pathway as a source of additional soil air might be an important contributor to the observed behavior. The high resistance to soil gas flow in the surrounding sandy clay soil does not allow for a very high flow of air from the atmosphere above the soil into the subslab region. Having a nearby source of air to support increased advective flow into the structure from the subslab region might be a contributor to increased contaminant entry, even if the pipe itself were not a source of contaminant. The model was re-run to reflect this possibility and the results are shown in Figure 3.13.

It is observed from the solid green line in Figure 3.13 that with the preferential pathway providing only “clean air” to the gravel sub-base, the model predicted results not very different from those when the preferential pathway was entirely closed off (in Figure 3.12). In other words, merely increasing the advective soil gas entry rate into the structure (which did happen) did not significantly increase the contaminant entry rate because in this case, the VI process was controlled by relatively slow diffusion of contaminant through the vadose zone.

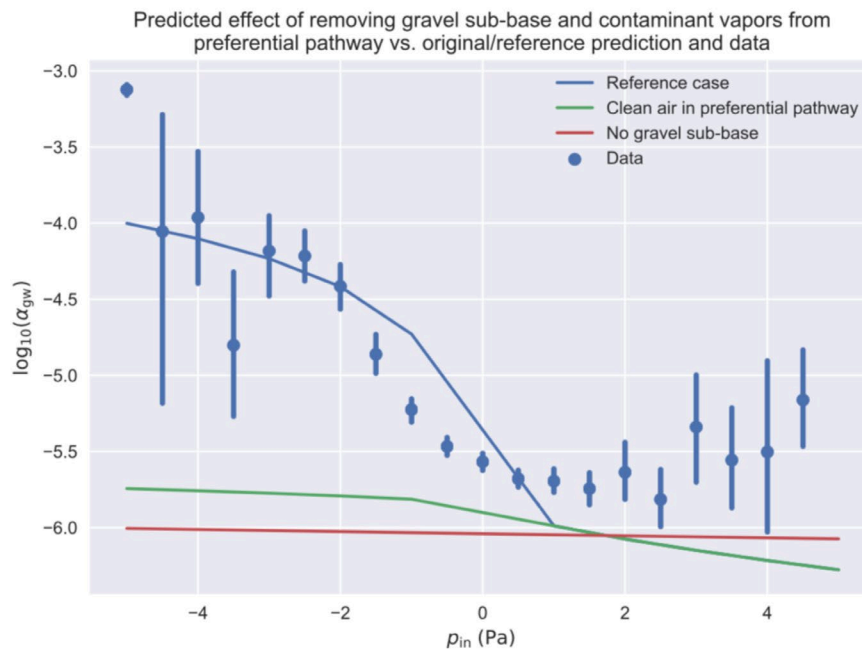


Figure 3.13. An Illustration of the Separate Influences of Preferential Pathway and Gravel Sub-base on Predicted Indoor Air Contaminant Concentrations.

Next, the influence of the gravel sub-base was examined. This case considered the situation when instead of dead-ending in a gravel sub-base, a pipe carrying contaminant vapors ends in soil (in this case, the sandy clay that was characteristic of the ASU study site). In terms of modeling the situation, this simply meant exchanging in the model the properties of the gravel layer for the properties of the surrounding soil. Again, the preferential pathway was a source of both air and contaminant in this case. The results of this calculation are shown in Figure 3.13 as the red line.

It may be seen that the elimination of the gravel sub-base dramatically decreases the predicted concentrations relative to the earlier predictions for when the preferential pathway exited into gravel (the blue line). In other words, delivery of contaminant vapor to the subslab region by the preferential pathway itself has very little effect, unless there is a highly permeable pathway for the contaminant to enter the structure. This also illustrates why the substantially increased indoor depressurization employed in the CPM technique will not necessarily always result in a significant increase in indoor air contaminant concentration- there may not exist the possibility of increasing advective entry rate because the surrounding soil cannot support increased airflow.

3.5 THE ROLE OF ADVECTION IN CONTAMINANT ENTRY

It is the complicated interplay of both contaminant and air supply to the foundation subslab region that very strongly determines the resulting contaminant entry rate, and therefore, the indoor air contaminant concentration at the ASU study site. The degree to which advective transport plays an important role in entry of contaminants into a structure can be considered by examining the Péclet number for transport through the foundation crack. The Péclet number has already been introduced in discussing the stability of the numerical solutions obtained using the FEM. Here, it is considered as a dimensionless parameter defined as the ratio of advective to diffusive transport rate across a characteristic length, which is here the length of the modeled foundation crack. For present purposes, the Péclet number is then defined as:

$$Pe = \frac{\text{Advection rate}}{\text{Diffusion rate}} = \frac{u_{ck} L_{slab}}{D_g} \quad (3.1)$$

where u_{ck} [m s^{-1}] is the airflow velocity across (through) the crack $L_{slab} = 15 \text{ cm}$ is the thickness of the foundation slab, i.e. the characteristic length for transport; and $D_g = 6.87 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ is the diffusivity of TCE in air. When $Pe \gg 1$, then the transport rate of contaminant through the crack is controlled by advection, whereas when $Pe \ll 1$ this indicates that the transport rate of contaminant through the crack is controlled by diffusion. If the contaminant transport through the crack is diffusion controlled, the indoor-outdoor pressure difference does not determine the contaminant entry rate, because advection (which is driven by the pressure difference) through the crack is not important.

Figure 3.14 shows how the Péclet number varies with indoor pressure level, for the cases considered in Figure 3.13. It is apparent that in this case, the entry of contaminant into the structure is generally dominated by diffusion, except at higher extents of depressurization in the presence of a gravel sub-base and preferential pathway. Absent either the gravel sub-base or the preferential pathway, the contaminant entry takes place through a relatively slow diffusion process, and its rate does not depend upon indoor pressure.

The important conclusion of this modeling exercise is that the mere existence of a preferential pathway delivering contaminants to some area outside of a structure is not sufficient to assure that it will have a significant impact on indoor air contaminant concentration. It is important how the delivery of contaminants to the vicinity of the structure is combined with the ability to advectively sweep them into the structure that determines the importance of the preferential pathway.

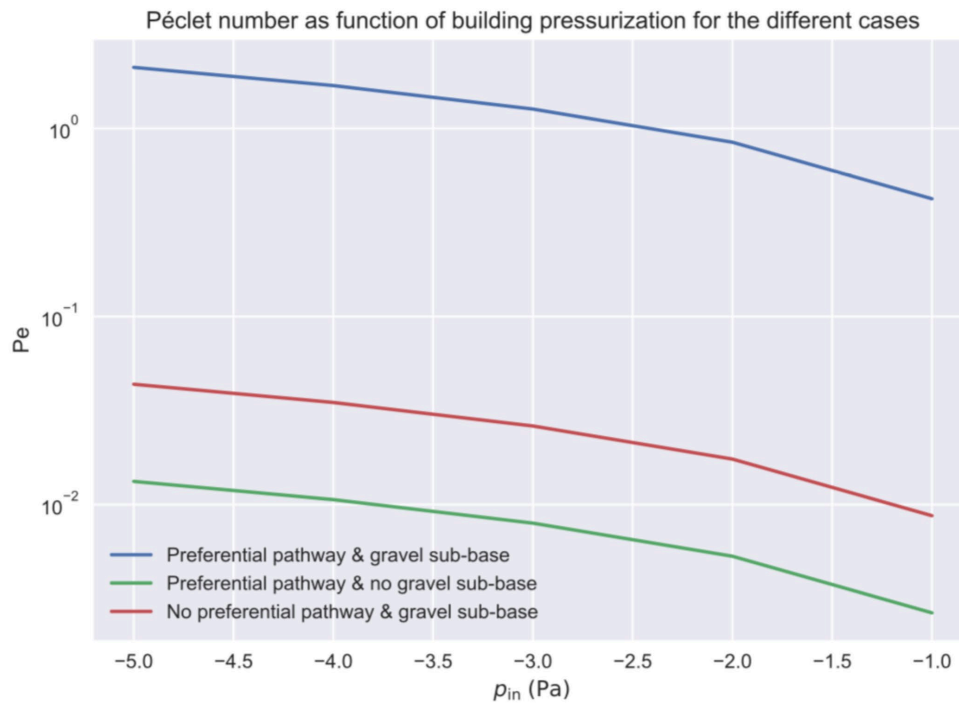


Figure 3.14. Péclet Number for Transport Through the Foundation Crack of the Modeled Structure as a Function of Building Indoor Pressure.

The blue curve shows the results of the calculations corresponding to when the preferential pathway delivers both contaminant and air to the gravel sub-base. The green curve shows the situation when the same preferential pathway dead-ends in sandy clay soil instead of gravel. The red curve shows a case in which there is simply a gravel sub-base, but no preferential pathway.

While the above analyses were all performed for steady state situations, the results are sufficient to substantially explain the observations of temporal variations in indoor air contaminant concentration at the ASU study site. The driver of the large temporal fluctuations must have primarily been fluctuations in indoor air pressure, acting on the unique combination of preferential pathway delivery of contaminants to the subslab and the existence of a highly permeable gravel sub-base that allowed their delivery to the indoor space via an advective mechanism. This is a rather specific combination of features that will not necessarily be present at many other VI sites, and leads to the conclusion that the ASU site was unusually configured (by its original construction) in such a way as to lead to the dramatic variations observed.

The above conclusion should not be construed as implying that only in the presence of a permeable sub-base and preferential pathway can significant temporal variation in indoor air contaminant concentrations be observed. Advectively controlled contaminant entry is apparent at some sites that do not have preferential pathways. A good example is provided by Naval Air Station North Island [25]. This site will be separately considered below in a broader discussion of the factors that control contaminant entry. There are, however, other factors not yet explicitly considered in the modeling that can also contribute to the temporal variation in indoor air contaminant concentrations. One of the most potentially important of these is air exchange rate.

3.6 CONSIDERING THE INFLUENCE OF INDOOR AIR EXCHANGE RATES

The simulations presented thus far have all assumed that the indoor air exchange rate is a constant 0.5 h^{-1} irrespective of any other factors, including the extent of house (de) pressurization. This is not entirely realistic, as air exchange rates in real structures constantly fluctuate and this is particularly so if the HVAC conditions change significantly with time. Any change in air exchange rate will have an impact on indoor contaminant concentrations, as is immediately apparent from equation 2.1. The concentration is inversely proportional to the air exchange rate.

To explore how air exchange rate influences predictions, model simulations were rerun assuming other realistic air exchange rates. Prediction of air exchange rate temporal variations is difficult, as they are influenced by building operation, indoor/outdoor temperature differences, wind, etc. Building air exchange rates are often regulated as part of local building codes, and depending on the type of building, typical values and bounds are more or less known. Here, a range of realistic constant air exchange rate values was examined. At the ASU study site, air exchange rates were measured using a tracer-gas study, and the obtained 10th, 50th, and 90th percentile air exchange rate values are shown in Table 3.1. Also shown are the corresponding values obtained from studies at the EPA duplex, and those from an independent EPA study that measured air exchange rates nationwide. Based on these values, the VI model was rerun using air exchange values of 0.1 , 0.5 and 0.9 h^{-1} .

Table 3.1. Observed Air Exchange Rates in h^{-1} .

Site		Percentile	
	10 th	50th	90th
EPA Study [77,78]	0.16-0.2	0.35-0.49	1.21-1.49
ASU Study Site [23,24]	0.21	0.43	0.78
EPA Duplex [74]	0.34	0.74	1.27

Figure 3.15 shows the result of varying the air exchange rates when predicting α_{gw} . The calculation shows the results from the same underlying model that was used to describe the behavior at the ASU study site. Here the central lines are the results corresponding to $A_e = 0.5 \text{ h}^{-1}$, while the upper and lower bounds of each shaded area correspond to $A_e = 0.1$ and 0.9 h^{-1} respectively. The shaded areas cover much of the observed spread in α_{gw} values. It is not surprising that given an almost order of magnitude spread in air exchange rates, the predictions of indoor air contaminant concentrations also show this magnitude of spread. This is why there is often observed an order of magnitude spread in measured indoor air contaminant concentrations, even absent the influence of any preferential pathway.

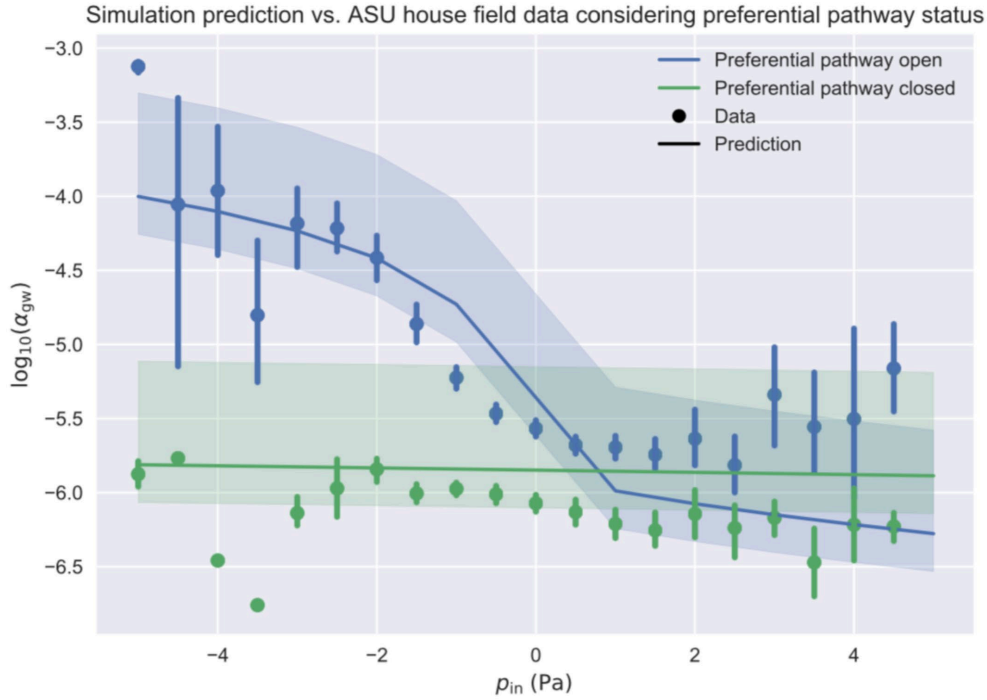


Figure 3.15. Modeling Result from Figure 3.12 but with Added Shaded Area Demonstrating the Effects of Assuming Different Air Exchange Rates.

The central lines are the result corresponding to $A_e = 0.5 \text{ h}^{-1}$, while the upper and lower bounds of each shaded area correspond to $A_e = 0.1$ and 0.9 h^{-1} respectively.

3.7 THE COMBINED INFLUENCE OF AIR EXCHANGE RATE AND INDOOR PRESSURE FLUCTUATIONS

While the influence of air exchange rate fluctuations was in some sense easily anticipated, given the direct linkage of indoor air contaminant concentrations and exchange rate, the situation becomes more complicated in the presence of fluctuations in more than one driver of the VI process. This is where the value of numerical models of the process becomes more obvious, since predicting the result of simultaneous variation in two key variables is much more difficult. As an example of how such modeling can provide insights, the situation at the ASU study site is reconsidered. At that site, typically both indoor air pressure and air exchange rate varied with time. The already presented numerical model is now implemented with the transient terms included in equations 2.39 and 2.40. Both the median diurnal variations of indoor pressure, p_{in} , and air exchange rate, A_e , are used as model inputs. Both of these variables were tracked over time, so it is possible to model a situation with actual time-dependent values of the two variables. The model predictions are explored both with and without the preferential pathway present corresponding to the land drain valve being open or closed, respectively. The median diurnal values of p_{in} and A_e taken at one-hour intervals over a 24-hour period were used. In order to achieve finer time resolution in these variables, the values were interpolated using cubic splines between the one-hour measurement points. Comparison is made to a case where only the median diurnal values of p_{in} and $A = 0.5 \text{ h}^{-1}$ were used.

Figure 3.16 shows the temporal variation of α_{gw} throughout the prototypical day. Again, the value of this attenuation coefficient is the indoor air contaminant concentration normalized by a source vapor concentration. When the preferential pathway is present, variability of α_{gw} , and thus indoor air contaminant concentration is driven by fluctuations in contaminant entry rate-- the predictions from the variable and constant air exchange rate cases do not differ much from each other. Both predict an almost order of magnitude variation in indoor air contaminant concentration driven by the very modest fluctuations in indoor air pressure. Note that when the indoor air pressure went only slightly negative, there was a substantial rise in concentration, but when the indoor air pressure was slightly positive from about 7 to 17 hours, the entry rate of contaminant greatly decreased and the indoor air contaminant concentration quickly responded.

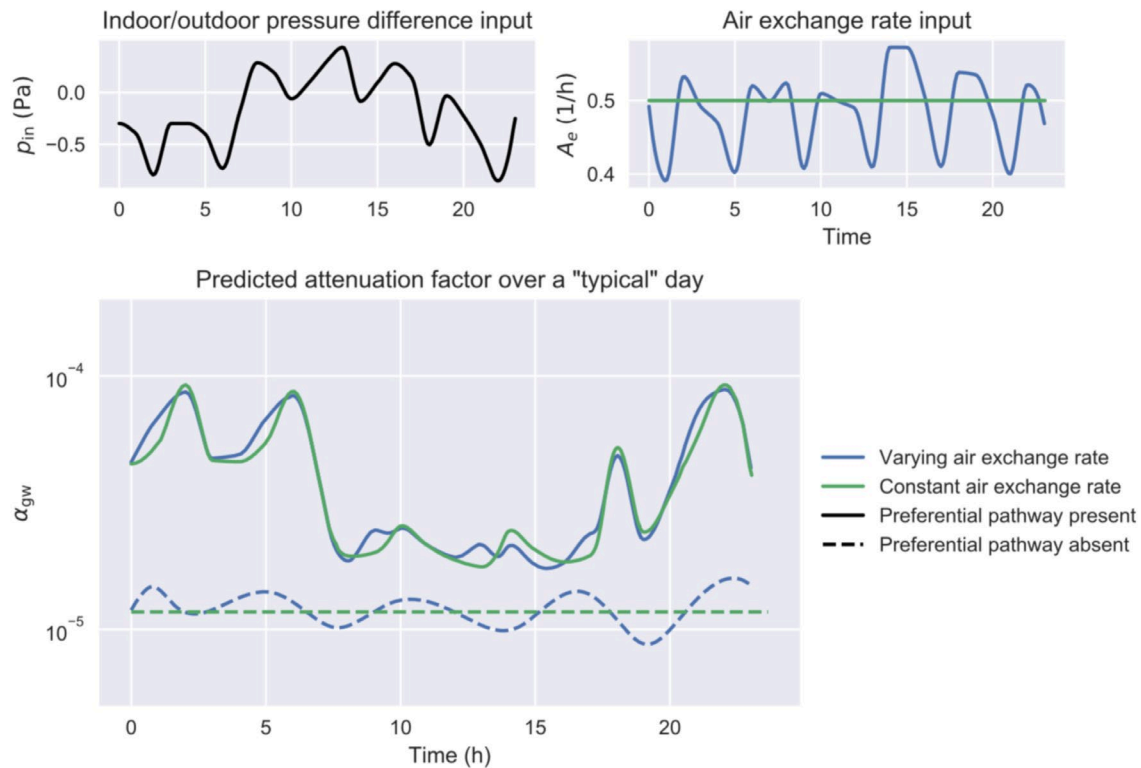


Figure 3.16. Predicted Indoor Contaminant Concentration (Represented as Attenuation from Groundwater) Over a “Typical” Day.

Here typical hourly median indoor/outdoor pressure difference and air exchange rates recorded at the ASU study site were used as inputs. For comparison, a case of constant air exchange rate (0.5 h^{-1}) is also shown. The preferential pathway was either “present” (corresponding to the valve being open) or “absent” (corresponding to the case in which it was closed).

When the preferential pathway was closed off, the model predicts virtually no variability of α_{gw} except for what is driven by the fluctuations in air exchange rate. In this case, as compared to that shown in Figure 3.15, the variability in air exchange rate was quite modest, so the response in predicted indoor air contaminant concentration is likewise quite modest. This is again because when the preferential pathway is not present, the delivery of the contaminant to the subslab is

driven purely by diffusion through the soil, and the very modest fluctuations in indoor air pressure have virtually no effect on the rate of that diffusion process.

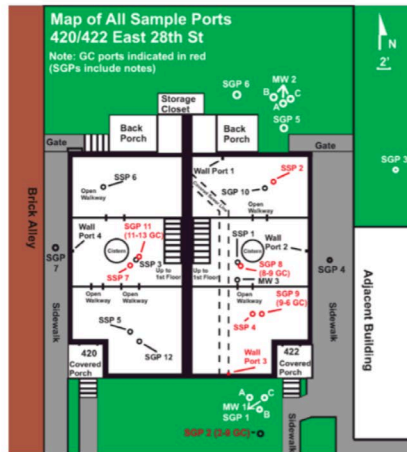
The predictions of the variability in indoor air contaminant concentrations were compared to those from the ASU study site. The predictions from this analysis were about a factor of 2 greater than what was observed at the site when the preferential pathway was open, but the predictions were almost exactly what was observed with that pathway closed. Thus, this very simple example of a transient calculation shows the ability of a numerical model of the VI process to quantitatively predict the influence of simultaneously varying parameters, something that is difficult to do by any other means.

3.8 THE COMPLICATED SITUATION AT THE EPA DUPLEX STUDY SITE

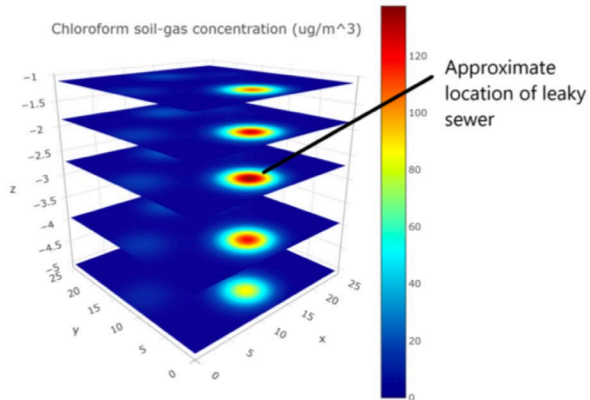
The modeling of the EPA duplex study site in Indianapolis presented more of a challenge, because of the less well defined role of a potential preferential pathway. This pathway was the ordinary sanitary sewer leading from the duplex to a main sewer line in the street before the house. The situation is shown in Figure 3.17. Based upon the soil gas measurements taken in front of the house, it appeared that the sewer was leaking vapors into the soil immediately adjacent to the structure. The spatial variability of the soil-gas contaminant concentration was investigated by interpolating the recorded data using the kriging technique, which is commonly used in geostatistics where sparse spatial data can be interpolated over a larger spatial grid [79]. The results of the kriging process are plotted in Figure 3.17. These are soil-gas contaminant concentrations each from a period that is (by inspection) determined to be relatively “representative” of the overall temporally separated dataset. The soil-gas contaminant concentrations actually fluctuate spatially in time, but what are displayed are general trends.

Figure 3.17 shows the variability for different contaminants observed at that site. In particular, trichloroethene (TCE) exhibits relatively minor spatial variability compared to chloroform or tetrachloroethene (PCE). A likely explanation for this disparity is the role that the sewer played at this site. In a later study of this site, McHugh et al. [22] found that PCE and chloroform could be found throughout the sewer network in the neighborhood whereas this was not true of TCE. In Figure 3.17, there is a “hot spot” in the middle slice, approximately at a depth of -2.75 m, roughly in the middle of the front lawn area. This is approximately the spot where the sewer line servicing the EPA duplex was located, which strongly suggests that there was a leak of vapors to the soil in that area.

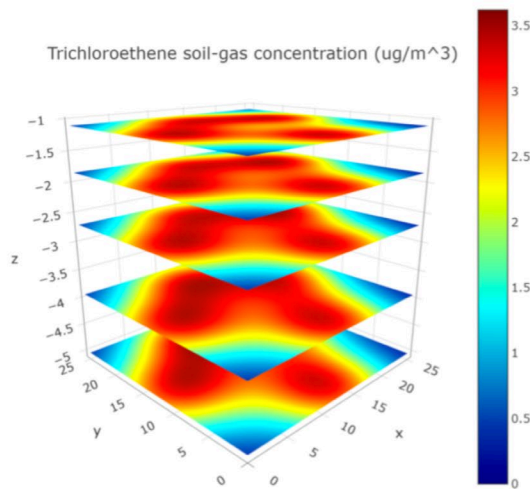
Unfortunately, the temporal aspects of the presence of contaminants in the soil, and how these related to indoor air contaminant concentrations were not easily relatable, so testing of the model against results at this site could not be performed in the same way as it was for the ASU study site. The kriging analysis merely provided time-averaged pictures of the soil gas profiles adjacent to the house, which would clearly need to be built into any model of transport into the house. The study by McHugh et al. [22] moreover offered a complicated picture of transport of these species in the sewer.



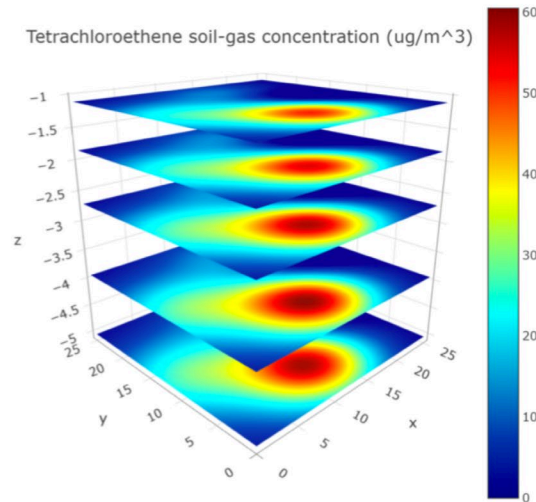
(a) Floorplan of the EPA duplex. The soil-gas figures x & y coordinates are relative to the bottom left corner.



(b) Soil-gas concentration of chloroform.



(c) Soil-gas concentration of TCE.



(d) Soil-gas concentration of PCE.

Figure 3.17. Interpolated Soil-gas Contaminant Concentrations for Chloroform (b), TCE (c), and PCE (d) Underneath and Adjacent to the EPA Duplex.

On the other hand, there is nothing even in this complicated scenario that would preclude development of a numerical model of the processes there. The contaminants would be modeled separately from each other, because they do not influence each other's transport (because they are so dilute). So as opposed to showing a preferential pathway that ends in the gravel sub-layer beneath the foundation slab (as in the case of the ASU site) here, the preferential pathway delivers the contaminant vapor to soil outside of the foundation. This leads to consideration of the importance of the soil through which the contaminant must be transported in order to reach the foundation, which topic is now considered.

3.9 THE ROLE OF SOIL PROPERTIES AND THE DOMINANT MODE OF CONTAMINANT ENTRY

The numerical modeling of VI described above has led to clear insights on some aspects of the process. One of these is the critical importance of the driving force for contaminant entry into a structure. There are two commonly accepted mechanisms by which contaminants can enter a building from the soil beneath it – advection and diffusion. In the case of advection, contaminant is carried into a building as a constituent of soil gas, which is swept into the building by a pressure gradient from soil to building interior. As already shown above in connection with Figure 3.16, such gradients need not be large and a few Pa can drive such a flow under the appropriate conditions. If the building is at neutral pressure relative to ambient, then there can be no advection, and only diffusion will move contaminants. On the other hand, if the interior of the structure is pressurized relative to the sub-foundation soil, then the advective flow will be out of the building, meaning that the flow cannot bring in contaminants from the subsurface. In a large structure that might be characterized by many different zones, it is possible that some portions of the building might be positive and other portions negative relative to the surrounding environment. This complication will not be considered further here, but in terms of modeling the process, there is nothing that prevents specifying boundary conditions at the foundation, which take this spatial variability into account.

Regardless of the existence or direction of a pressure gradient, there generally exists a contaminant concentration gradient from the soil into the structure, which means that there is always a driving force for diffusive entry of the contaminant into the building. It is only if the outward advective flow is high enough can this diffusive entry driving force can be overcome, and contaminant entry prevented. The very small pressure gradients that characterize many VI scenarios will often not lead to high enough advective flow rates to fully cut off the diffusive entry.

It needs to always be kept in mind that advective flow into a structure requires that the air (soil gas) be supplied from someplace. Ultimately, that source of air must be the ground surface. Advective transport at a VI site is only possible if there is a pathway that allows facile delivery of air (soil-gas) to the entry point in the foundation. Soil generally offers a large resistance to transport of soil gas bearing in mind that the pressure gradients available to drive flows are normally quite small. It has been shown in previous modeling studies that for quite comparable levels of contaminant vapor concentration beneath a foundation slab, very different indoor air contaminant concentrations may be realized, depending upon the ability of the surrounding soil to support advective flow [46]. This highlights the importance in vapor intrusion investigations of identifying features that will allow significant advective flow from soil to the building interior.

This leads to the further conclusion that only when advective entry is significant can use of building depressurization (in a controlled pressure method study) lead to significant enhancement of indoor air contaminant concentration. Depressurization will not significantly enhance the diffusion entry rate, because the pressure dependence of the diffusion coefficient in the range of relevance for VI is trivial. It is also only possible to see effects of weather (e.g., barometric pressure, wind, ground snow cover) on contaminant entry rates if the contribution of advection is significant.

Historically, the most widely held view of vapor intrusion has been that it is advective entry dominated, and indeed at many sites that is the case. But there are many examples that counter this view. For example, Hers et al. [80] continuously monitored pressure differentials at a VI site in Canada, and their data was used together with a reactive transport model (MIN3P-DUSTY) to simulate biodegradation and contaminant vapor transport at the site. They concluded that contaminant transport was dominated by diffusion, and that there was little relation between building depressurization and contaminant entry rate.

The modeling of the ASU site in this work helped to explain why building pressurization influenced indoor air contaminant concentrations much more before the closing off of the preferential pathway than after its closure. The preferential pathway provided not only the contaminant but also the air needed for advective transport of contaminant vapors through the foundation breach. It was shown that absent the preferential pathway, the soil surrounding the house itself presented too much resistance to airflow for this to be possible. Only one soil type was explored in that modeling -- sandy clay. This is a relatively impermeable soil, and leads to the question of whether other soils would lead to the same result. Furthermore, the modeled scenario featured a basement, in which the atmosphere is relatively far removed from the foundation breach. It is of interest to show how the assumption of a different kind of construction (slab-on-grade) might also influence the results.

The 12 soil types defined by the EPA (see Table B.1) were thus considered, and for each of these basement and slab- on-grade cases examined. For purposes of this modeling work, the depth of the bottom of the foundation slabs (located at 1 m and 15 cm bgs) defined the “basement” and “slab-on-grade” cases, respectively. Further, the building was assumed to be depressurized to $p_{in} = -15$ Pa, a value slightly greater than “normal”, in order to show more clearly the effects on advective entry potential. As before, the slab thickness was assumed to be a typical 15 cm, and the foundation crack width to be 1 cm.

It has already been shown in Figure 3.13 that a highly permeable gravel layer in the sub-slab region was of little importance in determining contaminant entry rate, absent an air source supplied by a preferential pathway. The results from that case were virtually indistinguishable from the case in which there was no gravel sub-base layer. This was because what limited the airflow needed to support advective entry was the resistance in the soil that surrounded the gravel sub-base. Thus, in considering the effects of different soil types on entry rate, there is no need to include a gravel sub-base in the calculations because it makes no significant difference.

The results of the calculations are shown in Figure 3.18 in terms of the Péclet number for the modeled contaminant entry pathway. This Péclet number has been previously defined in equation 3.1 as the ratio of advective contaminant entry rate to diffusive contaminant entry rate, with values of $Pe \gg 1$ indicating that advective entry dominates, whereas $Pe \ll 1$ indicates that diffusive entry dominates. Immediately apparent from Figure 3.18 is that for virtually all soil types except sand, advection is unlikely to control contaminant entry, even with the assumed significantly higher than normal indoor depressurization driving force. Most soils are too impermeable to allow sufficient airflow to be sucked into the building by the small pressure gradient that exists between the building interior and the subsurface. Sites characterized by sandy soil are the exception to this.

The implications of such a conclusion are significant for use of the controlled pressure method (CPM) for investigation of VI sites. If this technique is applied where the structure's foundation is surrounded by well-consolidated soil, it is unlikely that a significant increase in entry rate will be observed. It is important to recognize the assumption of "well-consolidated" soil in drawing this conclusion; if the soil adjacent to the foundation has been significantly disturbed such that its permeability is more like that of sand, this conclusion might not hold, particularly if there is a short-circuit path for air flow from the ground surface immediately adjacent to the foundation wall. On the other hand, this conclusion might hold for any soil type if the ground surface around the foundation is paved over or otherwise made impervious (e.g., by the ground surface being iced over).

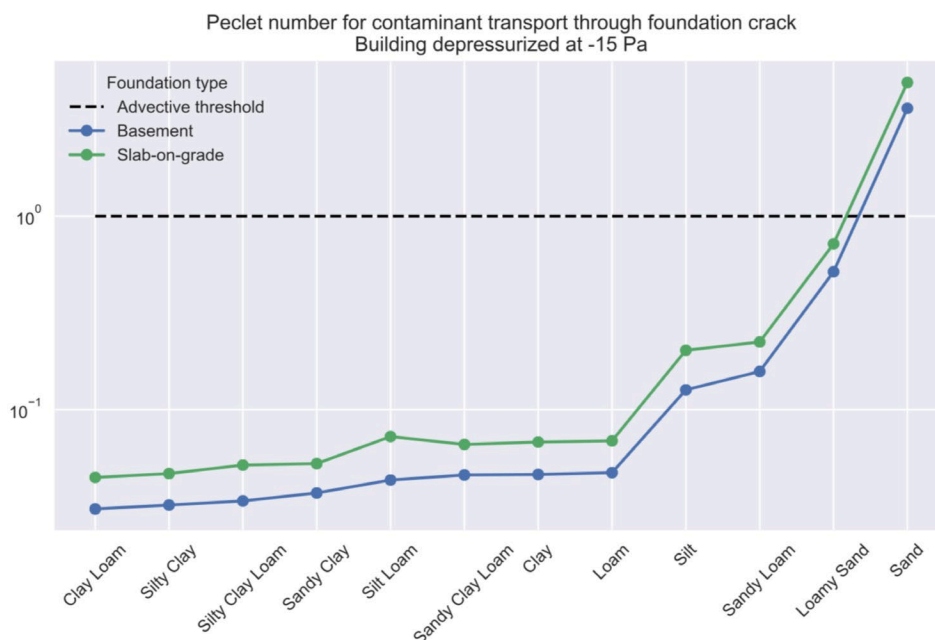


Figure 3.18. Predicted Effects of Soil and Foundation Types on the Contaminant Entry Peclet Number.

Pe = 1 is marked by the dashed line.

The above might help to explain the somewhat inconsistent results often obtained in investigations using the CPM technique [30, 31]- if there is not advective control of contaminant entry, the method will not increase the indoor air contaminant concentration. This is not a basis for abandoning the technique, but rather, CPM can be a way of showing that in a particular scenario the contaminant entry rate is definitively controlled by diffusion from source through the soil. The technique can therefore be used to identify scenarios in which a preferential pathway might be present.

The Case of Naval Air Station North Island

An illustration of the importance of soil type on determining VI behavior is provided by Naval Air Station (NAS) North Island near San Diego, California. This site is significantly contaminated by TCE. It is also characterized by sandy soil. In a detailed temporal study of this site, it was found that indoor air contaminant concentration and building pressurization were highly correlated [25]. Figure 3.19 illustrates this correlation.

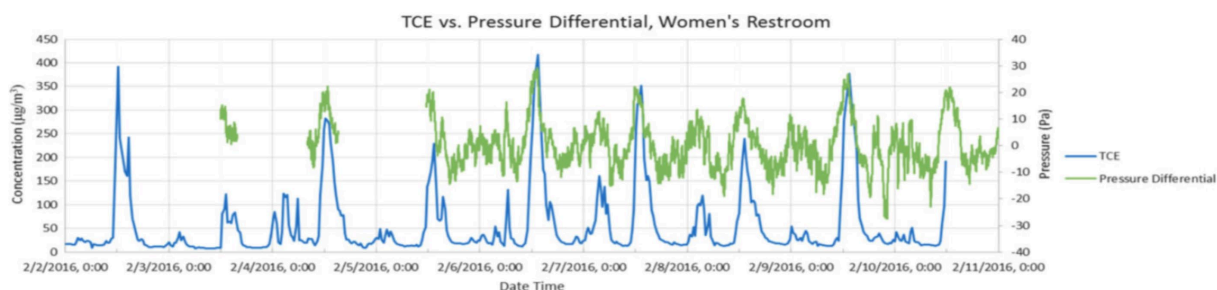


Figure 3.19. Time Series Data from NAS North Island [25].

In this case, positive values of pressure differential indicate a depressurization of the building relative to ambient.

There was no identified preferential pathway at NAS North Island, so the contaminant arrived at the building foundation via normal transport via the soil. Because the pressure dependence of the results is indicative of an advectively determined contaminant entry process, the only way this is possible is if the sandy soil characterizing the site was sufficiently permeable that it can support the needed airflow. This is generally consistent with the results of Figure 3.18, that show sandy soils allow such a result.

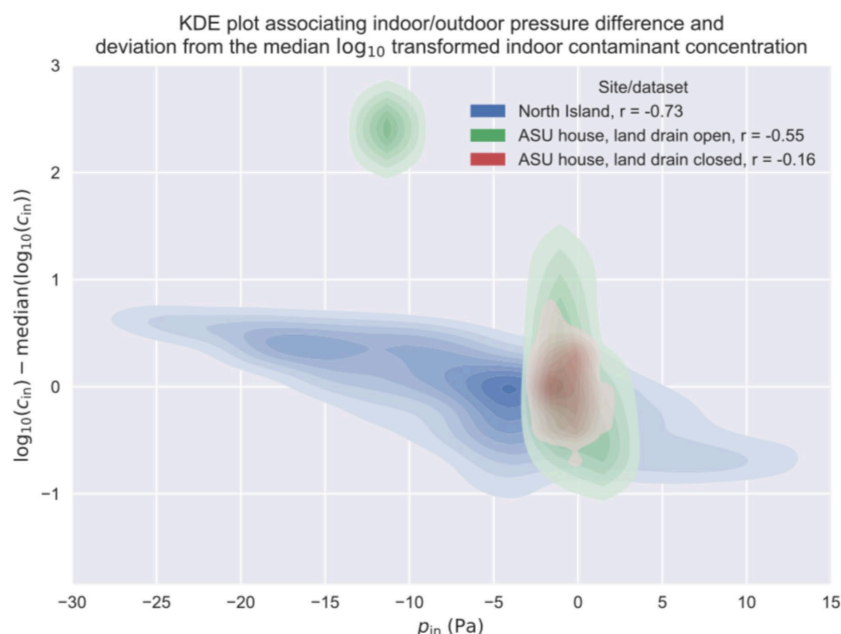


Figure 3.20. The Results of a Kernel Density Estimation (KDE) Analysis of Data from the NAS North Island and ASU Sites.

What is plotted on the abscissa is the distribution of measured indoor-outdoor pressure differences (negative values indicate indoor depressurization). The ordinate displays the distribution of indoor air contaminant concentrations, relative to the median value.

Further support for the existence of a fundamental difference between the NAS North Island and ASU sites is provided by Figure 3.20. This figure presents the results of a Kernel Density Estimation (KDE) analysis of the data on depressurization and indoor air contaminant concentrations at the two sites.

What is immediately apparent from Figure 3.20 is that the spread of pressure differentials observed at NAS North Island were considerably greater than those at the ASU site. In addition, NAS North Island is characterized by sandy soil. Thus, advectively mediated contaminant entry was favored both by the sandy permeable soil and the relatively high (for VI) pressure driving forces, which will increase the value of u_{ck} in equation 3.1. The result is that at NAS North Island a clear correlation is seen between the indoor air contaminant concentration and the pressure driving force, consistent with what was seen in Figure 3.19 (the Pearson r correlation coefficient shows this as well). On the other hand, at the ASU site, the observed distribution of pressure differentials is much narrower and much lower in magnitude. The correlation coefficient for the case of land drain closed operation confirms that there is virtually no relationship between indoor air contaminant concentrations and the pressure differential. Thus, the site was confirmed to behave in accord with diffusion-controlled contaminant entry when the land drain was closed.

The above results again caution that depressurization of a structure during CPM might not lead to the expected result of a significant increase in entry rate of contaminant. Proponents of CPM argue that the method offers a "worst possible case" result for a particular building, because the employed depressurization will be greater than anything that would naturally be encountered in the structure. This position is clearly influenced by a conceptual model that views advective entry as the dominant entry mode. The logic that such depressurization can offer a "worst possible case" result is not flawed, because enhancing contaminant entry rate is a real consequence of any depressurization. The only issue is the degree to which entry is enhanced. In a diffusive entry limited case—in such a case, there will be no apparent relationship between the degree of depressurization and entry rate (and thus, indoor air concentration). There is, however, an additional consideration when conducting a CPM investigation of VI -- CPM not only affects the contaminant vapor entry rate into a building, but can also have an impact on air exchange rates within the building being tested.

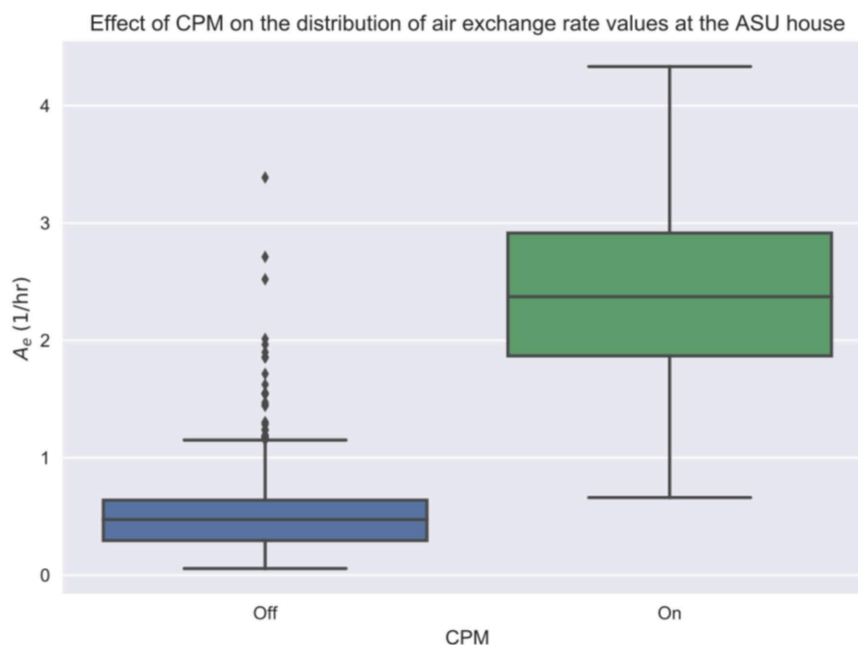


Figure 3.21. The Dependence of Air Exchange Rate on CPM Testing at the ASU Study Site.

Figure 3.21 shows the how during CPM air exchange rates increased significantly during the testing period. This will actually lead to enhanced contaminant expulsion from the house during the testing period, decreasing the indoor contaminant concentration relative to what it would be if only depressurization were involved. This may partially “mask” the effect of depressurization, a concern voiced with respect to such results [29].

3.10 THE INFLUENCE OF SEASON ON TEMPORAL VARIABILITY IN CONTAMINANT CONCENTRATIONS

Temporal variations in indoor air contaminant concentrations can occur on a variety of time-scales, from days to much longer seasonal variations. Figure 3.22 shows the seasonal variations at the ASU study site and the EPA duplex site.

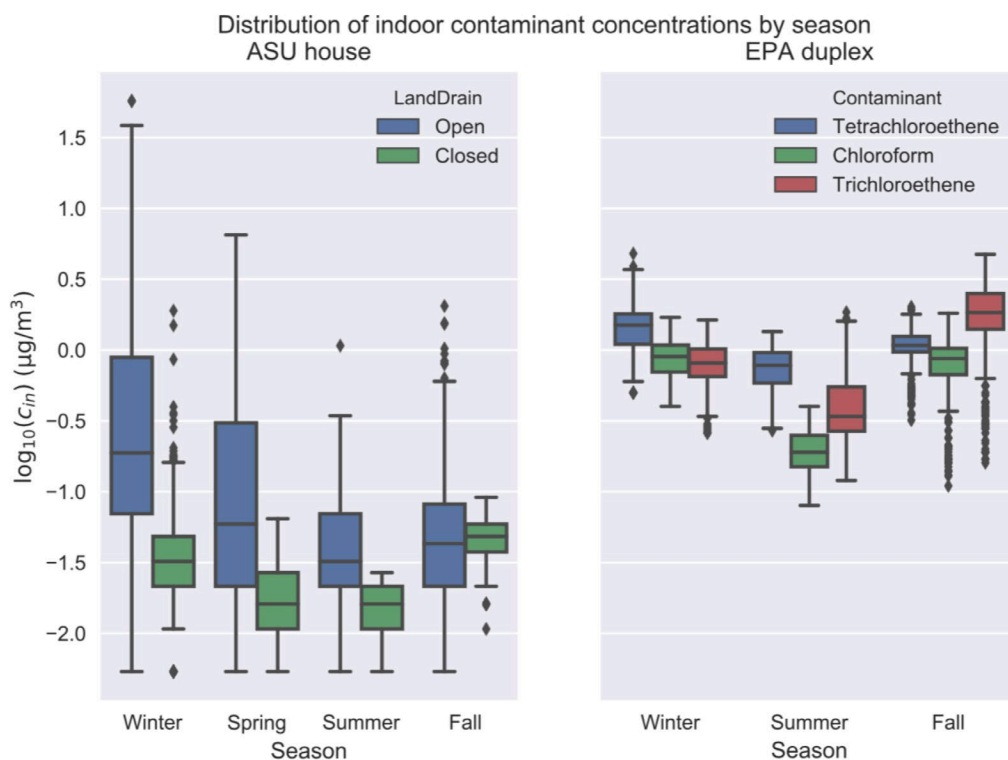


Figure 3.22. Seasonal Distributions of Indoor Contaminant Concentration at the ASU Site and EPA Duplex.

At the ASU house, the influence of the land drain preferential pathway is indicated. At the EPA duplex, the differences in observed distributions for three different contaminants are considered. Here “winter” includes December to February, with each subsequent season being defined by the subsequent three months.

Seasonal trends have been observed to be common at many VI sites, with winter often cited as the period most likely to lead to measurements of elevated indoor air contaminant concentrations [e.g., 8, 26, 80]. This general trend was observed at the ASU house when the land drain preferential pathway was open but was much weaker after the closing of the land drain. At the EPA duplex, indoor contaminant concentrations were slightly higher during winter and fall than summer, but only marginally so.

Figure 3.23 shows the measured variations in indoor-outdoor pressure differentials by season, for the ASU site and the EPA duplex site. It is apparent that the pressure driving force is as expected greatest during the heating season and in fact goes in the opposite direction during the summer season.

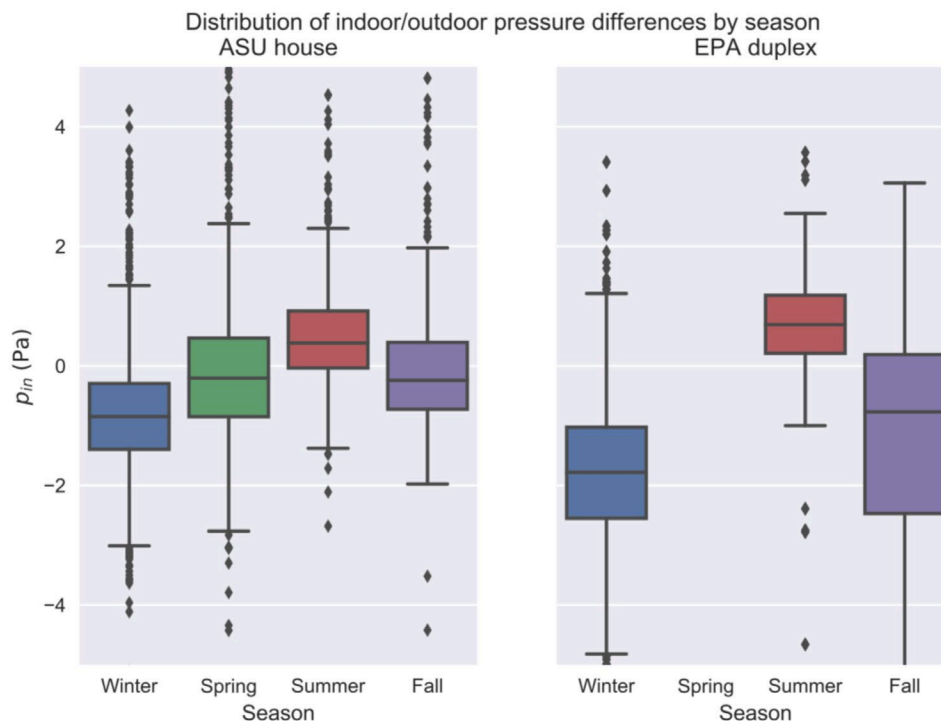


Figure 3.23. The Distributions of Indoor-outdoor Pressure Differentials by Season for the ASU Study Site and the EPA Duplex Site.

The implication of the data in Figure 3.23 is that there is likely to be a greater pressure driving force for advective entry of contaminant entry in winter. This is the basis for a preference for winter for performing indoor air sampling. But as has already been noted, this is based upon an advective controlled contaminant entry model that may often not be applicable. Since diffusion might often control contaminant entry, the “expected” effects of pressure may not be observed. In fact, seasonal effects may be confused by variations in air exchange rates.

Figure 3.24 is a KDE representation of differential pressure- air exchange rates from the data taken at the ASU study site. The heads of the arrows indicate the point most characteristic of any particular season. Consistent with what is shown in Figure 3.23, the most negative and positive pressure conditions are seen to exist in winter and summer, respectively. But very significantly, the air exchange rate most characteristic of winter was actually higher than that characteristic of summer. This fact would tend to counter any increased entry rate promoted by the greater depressurization in winter. Because when the preferential pathway was closed this was basically a diffusion-controlled entry site, the pressure differential would not have much of an effect. The air exchange rate would have a significant effect regardless of which mechanism controls entry, and these results suggest that summer conditions would tend to favor higher indoor air contaminant concentrations, all else being equal.

Thus, it may be misleading to look to winter as the “right” time to sample, in order to obtain the highest values of indoor air contaminant concentration, since that assumes a particular contaminant entry mechanism that may not be correct.

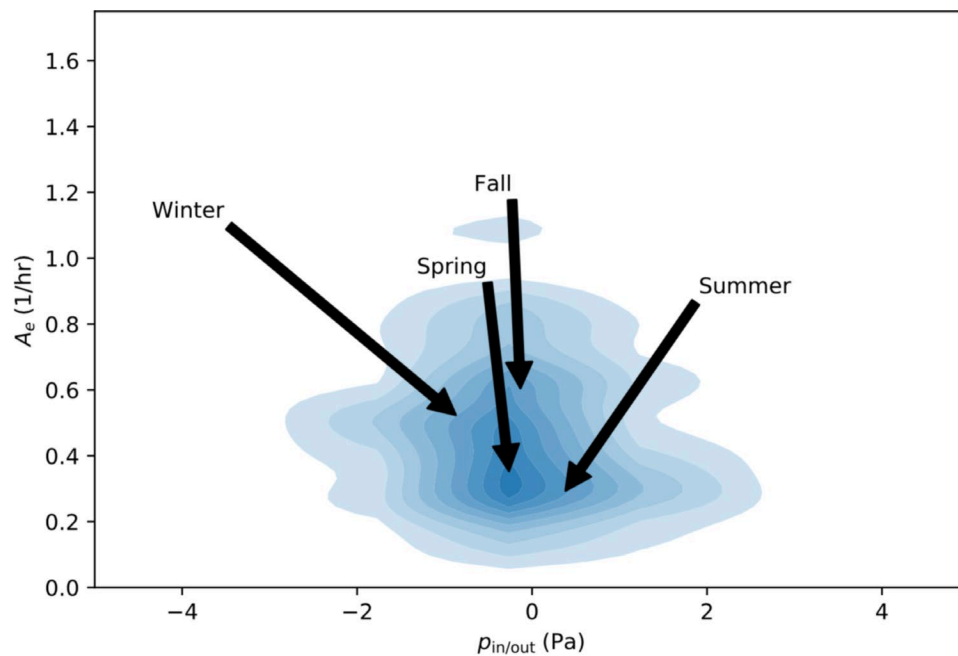


Figure 3.24. KDE Figure Showing Distributions and Relationship Between Indoor/Outdoor Pressure Difference and Air Exchange Rate from the ASU Study Site.

The seasonal median $p_{in/out}$ and A_e are shown. Only data from the non-CPM testing period were included.

4.0 MODELING VI WITH ADSORPTION PROCESSES

Most vapor intrusion (VI) contaminants have the capacity to sorb onto soil and common indoor materials, but the role and more importantly, the consequences of these sorption processes in VI are poorly understood [14,15,81]. The migration of contaminant vapors from their source into the VI impacted building and potential indoor sources is usually the prime concern in VI investigations. Rarely are the sorbed contaminant vapors in the soil or indoor considered in an investigation. These may potentially act as a capacitance, storing and releasing contaminant vapors in response to a change in contaminant concentration. Consequently, contaminant vapors may be more persistent than expected at a site that has undergone remediation, potentially reducing the effectiveness of mitigation in the short term, or leading to misleading results regarding mitigation efficacy.

It is well recognized that materials have the capacity to sorb pollutants. The sorptive capacity of various volatile organic compounds (VOCs) of concern in VI has been examined on a variety of building materials, such as particleboard [82], gypsum wallboard [83], and plywood and carpets [84]. However, most of these studies used relative high contaminant concentrations, usually at mg/m^3 levels [82] or even higher. This is several orders of magnitude higher than the concentrations relevant in VI and due to the often non-linear nature of sorption with respect to concentration, sorption studies at lower concentration are needed. Many studies have focused on the interaction between building materials and formaldehyde [84], toluene, and decane [84]. However, one of the contaminants of greatest concern in VI - trichloroethylene (TCE), has not received attention. This is despite the fact that sorption of TCE (and other comparable VOCs) on activated carbon is extensively used to treat indoor air contamination and their sorption on passive tube samplers is widely employed for analysis of these compounds [7].

The potential impact of sorption could perhaps be most significant in situations in which contaminant entry rates vary widely with time. If building indoor materials have high sorptive capacities, then desorption and adsorption processes may significantly affect the measured indoor air contaminant concentrations. Likewise, a significant amount of sorbed contaminant may be released from interior materials over an unknown period of time after mitigating the contaminant intrusion at a site. To help establish whether such processes play a significant role in a particular scenario, the use of numerical modeling can be helpful. This requires adding to the earlier model the effects of any suspected partitioning processes.

Modifying the Model

The same basic three-dimensional transient numerical model of a building overlying a TCE contaminated groundwater source as developed in section 2 may be used. The sorption processes do not affect the equation (Darcy's Law) used to describe soil gas flow in response to the pressure gradient induced by indoor depressurization, nor do they affect the boundary or initial conditions for that equation. Thus, equation 2.39 can still be used for this analysis, and it is unchanged.

Contaminants in the vadose zone now exist in three phases - gaseous, dissolved in water, and adsorbed onto soil particles. All of these must be accounted for by using equation 2.40 to model species transport in the vadose zone. Whereas earlier the term involving K_p , which describes adsorption to the solid phase (equation 2.41), was ignored, now it must be accounted for.

An initial condition must be provided for all concentration variables. For simplicity, the approach used here was to run the model for a relevant steady state case, and use the variable values obtained from that as a starting point for the transient analysis.

The processes of contaminant entry through the crack also remain as they were before. Once again, it is possible that either advection or diffusion of contaminant may govern the entry process.

What must change is the calculation of the indoor air contaminant concentration, since now sorption to indoor building materials must be accounted for. Hence the governing equations now become:

$$V_{bldg} \frac{\partial c_{in}}{\partial t} = n_{ck} - A_e c_{in} V_{bldg} - r_{sorb} V_{mat} \quad (4.1)$$

$$V_{mat} \frac{\partial c_{sorb}}{\partial t} = r_{sorb} V_{mat} \quad (4.2)$$

$$r_{sorb} = k_{ads} c_{in} - k_{des} c_{sorb} \quad (4.3)$$

Here V_{bldg} and V_{mat} are the relevant indoor building volume and volume of indoor material in m^3 ; c_{in} and c_{sorb} are the indoor and sorbed (onto the indoor material) contaminant concentrations in mol/m^3 ; n_{ck} is the contaminant entry rate in mol/s , which is calculated by integrating the contaminant flux j_{ck} over the foundation crack area; r_{sorb} sorption rate in $mol/(m^3 \cdot s)$; k_{ads} and k_{des} are the adsorption and desorption rate constants in $1/s$. The equilibrium constant for adsorption onto an indoor material is related to these latter two quantities:

$$K_p = \frac{k_{ads} c_{in}}{k_{des} c_{sorb}} \quad (4.4)$$

It should be noted that the significance of V_{bldg} is as it has been throughout the earlier part of this report, whereas V_{mat} now accounts for the amount of material in the building that can participate in adsorption (or absorption) of the contaminant. The choice to represent this in terms of material volume rather than material mass was arbitrary, but it permits maintaining consistent units for both vapor and sorbed concentrations.

Sample Results- The Effect of Contaminant Adsorption by Soil

The effect of abrupt changes in building depressurization, such as might be involved in CPM testing, was modeled. The initial condition for the simulation was a typical 5 Pa indoor depressurization. At the start of the simulation, the building was further depressurized to -15 Pa, and the simulation modeled the response over the course of 72 hours. For each of these cases, the simulation was run using two different soil types - sand and sandy loam. Sand was assumed here to not sorb any TCE, while for sandy loam a range of sorption isotherms were assumed, ranging from no sorption ($K_p = 0$) to a value experimentally determined for Appling soil ($K_p = 5.28 m^3/kg$).

Examining the experimentally determined isotherm value, the ratio between sorbed concentration and soil-gas phase concentration is 7708, i.e. there is a much larger amount of contaminant sorbed to the soil than present in the vapor phase of the vadose zone. Figure 4.1 shows the results of the simulations using the above limiting soil adsorption coefficient values and a range of values in between.

The top panel of Figure 4.1 effectively shows the indoor air contaminant concentration response. It was plotted as an attenuation factor, defined by:

$$\alpha_{gw} = \frac{c_{in}}{c_{gw} K_H} \quad (4.5)$$

This is done simply to scale the results to any source strength. The results in the top panel immediately reconfirm the importance of soil type in any pressure variation scenario. Highly permeable sand shows an immediate and significant increase in indoor air contaminant concentration, because contaminant entry is advectively controlled. All of the sandy loam cases show much more limited response to a pressure change, because the soil is relatively impermeable, and contaminant entry is diffusion controlled. Consequently, the system cannot respond very quickly, since there is no quick sweep of contaminants from soil into the structure. The effect of adsorption on soil is then likewise only modest as concentration gradients cannot change very quickly.

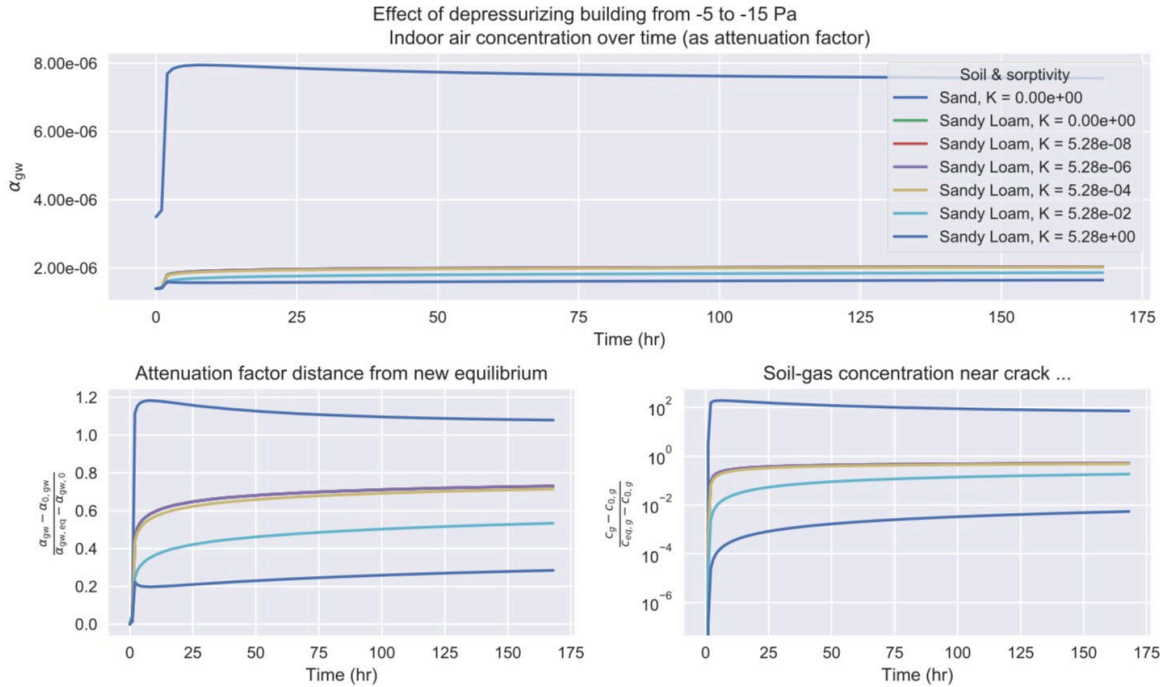


Figure 4.1. Simulations Showing the Influence of Contaminant Adsorption on Soil.

The top panel shows the impact on indoor air contaminant concentration (displayed as an attenuation factor relative to source). The lower left panel shows the time needed to approach the new equilibrium value, and the lower right shows the response of the absolute contaminant concentration adjacent to the foundation.

Despite the fact that for the values of adsorption coefficient selected the impact on indoor air contaminant concentrations is very limited, it is still instructive to examine the time scale for adjustment to a new equilibrium. The bottom left panel shows the time needed for indoor air contaminant concentration to reach a new equilibrium value as a fractional approach to that new equilibrium. At the start of the simulation, the building starts at an attenuation value of $\alpha_{gw,0}$, representing the steady-state indoor contaminant concentration when the building is depressurized to -5 Pa. As the building is depressurized to -15 Pa at $t=0$, the indoor air concentration approaches a new equilibrium state $\alpha_{gw,eq}$. Thus, despite the small extent of response, this scaling highlights for the sandy loam cases how long it takes to achieve the new equilibrium state. It is observed that there is a very fast initial response, but then the time required to reach the new steady state is quite long (hundreds of hours, the graph cannot display the very long times needed). This is because the time scale for the diffusion and adsorption processes in the soil to re-equilibrate is very long, as determined mainly by the low diffusion coefficient of contaminant in the vadose zone. The slowest adjustment to a new equilibrium is shown by the lowest curve, corresponding to the highest soil adsorption coefficient (that which is most realistic for this type of soil).

The results of the same simulations are shown in the bottom right panel as well, but this displays the average soil-gas concentration within a 5 cm diameter cylinder that surrounds the entire perimeter crack, representing the “inventory” of gas phase contaminant that is ready to enter the building. While the choice of 5 cm is arbitrary, this helps illustrate what happens in the near- foundation-crack region. Consistent with the long timescales observed for the indoor air to “adjust” to a new condition, the soil shows a similar slow adjustment. Again, the soil with the highest adsorption coefficient value shows the slowest response. This is entirely consistent with the soil of the vadose zone serving as a “capacitance” in the VI process. This has to do with the relative magnitude of the terms in the retardation factor, R , defined in equation 2.41. The condition that defines when the different curves for sandy loam diverge from one another is:

$$\rho_b K_H K_{ads} > \theta_w + \theta_g K_H \quad (4.6)$$

This occurs when $K_{ads} = 5.28 \cdot 10^{-4} \text{ (m}^3/\text{kg)}$, a point at which the ratio of adsorbed and soil-gas inventories at any point are roughly equal. It is at this point that the contaminant transport, i.e., replenishment from the source in the soil, starts to become significantly retarded by the adsorption sink. Under typical VI conditions, the ratio of $\theta_w + \theta_g K_H$ to $K_{ads} \rho_b K_H$ can vary by orders of magnitude, mainly depending upon the value of K_{ads} . Thus it may be difficult to generalize the influence of soil adsorption in VI scenarios, even though in the example here for a realistic soil value, that influence is very modest.

Sample Results - The Effect of Contaminant Adsorption by Indoor Materials

For these simulations it was assumed that there is no soil sorption, and that the soil is sand. It is further assumed that the walls of the usual 10 m by 10 m by 3 m basement (the indoor air space) are entirely made of one particular material of a certain thickness or depth that the contaminant can penetrate. This provides a certain volume or mass of adsorbing material in the indoor environment. This approach allows making a crude estimate of the influence of some materials. Table 4.1 shows the assumed thicknesses and resulting volumes of potentially adsorbing materials.

Material	d_p (mm)	V_{mat} (m ³)	$K_{ads}\rho_b$
Cinderblock	5	1.6	41,500
Wood	1	0.32	141
Drywall	10	3.2	215
Carpet	10	3.2	226
Paper	0.1	0.032	2196

Table 4.1. The Assumed Contaminant Penetration Depth and Calculated Volume of the Adsorbing Indoor Materials.

The material surface area is assumed to be the same, and each material completely covers the surfaces of the 10x10x3 meter room. Adsorption capacities determined by Shaui Xie, Brown University.

Once again, the modeled building is assumed to have been depressurized at -5 Pa at an initial steady-state and then is depressurized to -15 Pa. In this case, the building is assumed to then be pressurized to 15 Pa, and finally again depressurized to -5 Pa. For each step of the pressurization sequence, the new pressure is maintained for 24 hours. This pressurization cycle may be seen in the top left panel of Figure 4.2. This choice of pressurization cycle is arbitrary, but it is used to represent limiting cases of natural indoor pressure variations, or those artificially induced in CPM.

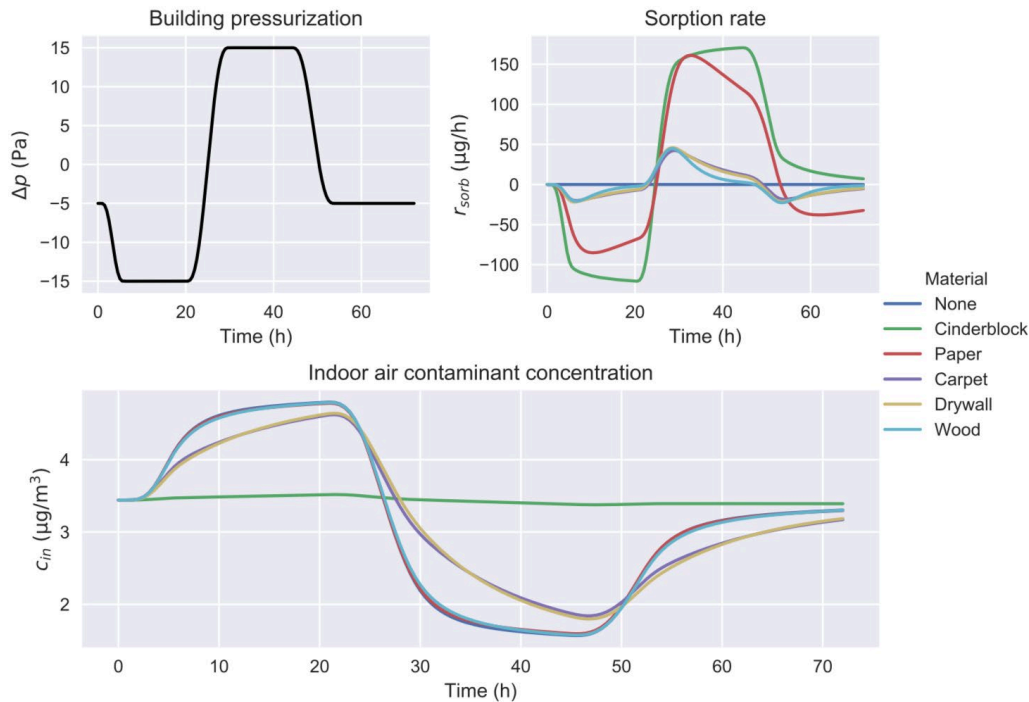


Figure 4.2. Simulation of Vapor Intrusion with Adsorption Onto/ Desorption from Various Indoor Materials.

The top left panel shows the pressure sequence and the top right panel shows the rate of adsorption and desorption. The bottom panel shows the effect on indoor air contaminant concentration.

The blue line is the reference case in which there is no sorptive material present in the structure. This line overlaps those for the wood and paper, which have only modest sorptive capacities. The presence of cinderblock, which contains a small amount of highly adsorptive carbon has a very significant effect, dampening out almost any change in indoor concentration. Drywall and carpet significantly delay the rate of change in the indoor concentration, but at the end of each 24-hour cycle, roughly the same indoor contaminant concentration is reached achieved as in the no sorption reference case. As the top right panel shows, paper responds quickly, but because of its low sorptive capacity, ultimately has little effect. Drywall and carpet respond slowly, but have a greater capacity and so can influence the system response more.

The significance of such results may be felt in certain types of processes. For example, if the CPM technique is used to study the response of the indoor air contaminant concentration, these results raise a question as to when might be the “right” time to sample indoor air concentrations. These results also serve to warn that some buildings might show very long times to respond to certain types of mitigation efforts, whereas others might respond quickly.

5.0 CONCLUSIONS

5.1 PROJECT GOALS

This project had two main goals. The first was to use numerical modeling as a tool to shed new light on the alarmingly large temporal variations in indoor air contaminant concentrations, observed at several well-studied vapor intrusion sites. These sites included the ASU study site outside of Hill AFB in Utah, the NAS North Island site in California and the EPA duplex study site in Indiana. It had already become apparent prior to this project that at the ASU site the explanation had to be related to the existence of a preferential pathway discovered after that investigation began. On the other hand, there was no known preferential pathway at the NAS North Island site, and investigation of a suspected preferential pathway at the EPA site took place during the time of this project. This still left an incomplete picture of the essential elements required for observing large temporal variations in indoor air contaminant concentrations at VI sites. Numerical modeling has been used to shed light on the processes that dictate the temporal variability.

The second aim of this project was to provide a manual that can be used by those who wish to engage in numerical modeling of VI sites. Here, the goal was to provide a roadmap that would allow use of standard, off-the-shelf software and desktop computing hardware to perform such modeling. The intent was to remove obstacles associated with use of custom or proprietary software for this purpose. In the VI investigation field, there is criticism that models have never been fully validated against actual sites. This is a valid criticism, in that such validation requires significant effort to collect enough input data that are difficult to obtain, even at the well-studied sites that are the subject of this work, let alone at the typical VI investigation site. Despite this, the claim has almost invariably also been made that modeling can represent a valid line of evidence alongside other site investigation data. It is in this spirit that the models offered in this project were developed. These models can be used as a check on site conceptual models since they will very readily point to where unwarranted physical assumptions are being made. An example of this is in the emphasis in this report on use of building depressurization in an effort to identify a “worst case” VI scenario. It is shown that this technique is only valid under a particular advection-controlled contaminant entry scenario, which cannot be assumed to exist under all conditions.

The project goals were achieved. The second goal (of providing a manual for those who wish to use detailed numerical modeling to examine vapor intrusion scenarios) has been achieved as originally envisioned; this document is such a manual and we believe can serve to guide those who will look to numerical modeling as a way of better understanding the response of real sites.

The first goal of the project was achieved, but in a way that was a bit different than had been originally envisioned. The model was successfully used to point to the key factors driving many order of magnitude variations in indoor air contaminant concentrations, and showed why different sites exhibited such significant variability despite very different physical conditions. What was not initially anticipated was how a simple metric of model performance based on prediction of indoor air contaminant concentrations was unrealistic, given the fact that the field data needed to make such a comparison would not generally be available. As discussed in section 3.4, this did not, however, limit the utility of the model in pointing to the conditions that will lead to such variations, and even to predictions of how large the influence of the key variables can be.

5.2 MAIN PROJECT CONCLUSIONS

- The large variations in measured indoor air contaminant concentrations at the ASU site had their origins in the existence of a combination of a preferential pathway combined with a ready source of air supporting advective entry of contaminants into the building. Absent either factor, there could not have been nearly as large a variation.
- The large variations in the indoor air contaminant concentrations at NAS North Island did not involve a preferential pathway, but were driven by an unusually high indoor depressurization in the presence of a permeable soil.
- Results from the ASU site suggest that variations of an order of magnitude in indoor air contaminant concentrations should be expected simply on the basis of the combined effects of air exchange rate and indoor depressurization effects.
- The generally assumed dependence of indoor air contaminant concentrations on the extent of indoor depressurization will not always be observed, if the entry rate of contaminant is diffusion controlled, as might be expected at many sites. This may limit the value of controlled pressure measurement characterizations of vapor intrusion potential. This might also be viewed as challenging the assumption that cold-season indoor air sampling will always lead to the most conservative result.

5.3 CONCLUSIONS REGARDING THE FACTORS DRIVING LARGE TEMPORAL VARIABILITY IN VI

The numerical modeling results that captured most of the salient features of the ASU site has shown that this site was characterized by a particular combination of factors that led to the large temporal variations observed only while the preferential pathway was open. It was the combination of the preferential pathway delivering contaminants to a highly permeable foundation sub-base together with that same preferential pathway delivering air that could support advective entry of contaminants, which was critical. Either factor alone would not have been sufficient to support the very large fluctuations in indoor air contaminant concentration.

The results from NAS North Island showed that the above combination of factors would not be necessary in all cases. There was no preferential pathway at North Island. But what was the same was the fact that there was a relatively permeable soil beneath the foundation, which could support the advective entry of contaminants from the soil. In the case of North Island, the pressure driving force for advective entry of soil gas was much larger than that at the ASU site. The feature that these two sites had in common was a permeable soil or foundation sub-base that would permit advective movement into the building of contaminants with soil gas.

Unfortunately, the results from the EPA study site did not lend themselves to development of an unambiguous model for that site. There was clearly delivery of contaminants to the site by a sewer pathway. The main effects of this pathway were, however, unclear. The data show that there was release of contaminant vapors from the sewer to the soil adjacent to the building, but whether this was the only entry pathway associated with the sewer could not be determined.

The modeling of the variability in indoor air contaminant concentration needed to explain why there was still the observation of almost order of magnitude variability in this quantity, even when a preferential pathway was not present. This variation was not really attributable to the soil transport portion of the vapor intrusion model, but rather, to the normal variability in air exchange rate. This is of course why some investigators prefer to discuss VI in terms of contaminant entry rate rather than indoor air concentration. Still, since the results of vapor intrusion modeling will invariably be compared to indoor air contaminant concentrations, it is important that the calculation at this final step of modeling be properly handled, by recognizing the need for good air exchange rate information at the location (the particular portion of the building) that is being modeled.

The modeling of transient phenomena related to adsorption of VI contaminants to soil and to indoor materials has indicated that both processes are characterized by long time scales for re-equilibration. The magnitudes of the effects did not appear to be very large, for the cases examined here, but because of the variability in materials and soils at different sites, it is unclear that this will always be the case.

5.4 A NEW TAXONOMY OF VI SITES

During the course of this work, it became apparent that there was an important distinction between certain kinds of VI sites that has not been fully developed within the research community interested in this topic. Simply put, the distinction is between sites in which the entry of contaminants into the building of interest is controlled by advection vs. diffusion. It is only in the case of buildings for which advection controls entry that indoor pressure (induced by the “stack effect” or induced during testing by controlled pressure methods) is important. Advection requires a pressure driving force, so the connection between these is apparent. But what seems to often have been a working assumption in VI investigations is that advection is significant in most cases. The results of this modeling study warn that in fact, most consolidated soils do not have a sufficiently high permeability to support significant advection under the small pressure driving force conditions present at most sites. This can be exacerbated by the presence around the building of paving, frozen ground, etc. which prevents the atmospheric source of the air needed for advection from doing so. In such cases, the sites can be characterized as diffusion entry rate controlled.

The significance of the above conclusion is that correlations between indoor air contaminant concentrations and the extent of indoor depressurization may not always exist. This in turn has implications regarding the recommendations for performing indoor air sampling in winter, when the stack effect might be greatest. At a diffusion entry controlled site, this might not be appropriate. In fact, it might make more sense to look for towards the season in which air exchange rates are lowest, which might be summer. The other implication of this conclusion is that the controlled depressurization of a building in a hunt for the “worst possible case” concentration might not lead to significant increase in indoor air contaminant concentrations, because in a diffusion controlled contaminant entry scenario, the rate of entry will not be impacted by depressurization. This does not in any sense invalidate the use of this kind of testing, since a result that shows a lack of sensitivity to depressurization will definitively indicate a diffusion rate controlled entry case, in which seasonality and weather effects are less likely to play a role in determining entry rates.

Again, the above conclusions came to light as a result of modeling typical conditions. They echo other earlier, similar conclusions that were anecdotal in nature, based upon observations at particular sites. The fact that these conclusions were not a-priori obvious is a testament to the complexity of the VI process, in which subtle aspects unique to particular sites can have significant consequences. This speaks again to the value of having a straightforward to use modeling tool, that can capture key features of a site and that can indicate when an unusual situation needs to be looked for.

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APPENDIX A GEOMETRY GENERATION EXAMPLE

To create the quarter domain geometry, only a few simple geometric objects and Boolean operations are required -- two cuboids, two rectangles, one Boolean difference operation, and one Boolean join operation. Figure 2.5 shows the resulting geometry. Note that $z = 0$ m is the groundwater/soil interface and the plane of symmetry is around the $(x, y) = (0 \text{ m}, 0 \text{ m})$ axis.

To create the soil surrounding the building using the COMSOL geometry generator:

1. Create a 15 m by 15 m by 4 m block with its base at $(x, y, z) = (0 \text{ m}, 0 \text{ m}, 0 \text{ m})$. This is the entire soil domain.
1. Create a 5 m by 5 m by 1 m block with its base at $(x, y, z) = (0 \text{ m}, 0 \text{ m}, 3 \text{ m})$. This will represent the volume that the house takes up in the soil, i.e. the underground portion of the basement.
2. Perform a difference operation, removing the “basement” block from the “soil” block.

At this point a quarter soil domain has been created, with an empty space that represents a house with a foundation slab located 1 m bgs.

The foundation crack will be modeled by joining two 1 cm wide strips that span the perimeter of the surface that represents the house foundation. These strips are created by joining two rectangles on the foundation surface. This is done by defining a work plane 3 m above zero. This allows placing two-dimensional objects on the surface of or inside a three-dimensional object.

1. On the work plane create a 5 m by 1 cm rectangle with its base at $(x, y) = (0 \text{ m}, 5 \text{ m} - 1 \text{ cm})$. This represents one side of the perimeter crack.
2. Copy the rectangle and rotate it 90° around the corner of the foundation, i.e. $(x, y) = (5 \text{ m} - 0.5 \text{ cm}, 5 \text{ m} - 0.5 \text{ cm})$.
3. Join the two rectangles to create a unified perimeter foundation crack.

With that, the geometry for the example VI scenario is complete.

APPENDIX B SOIL PROPERTIES

Table B.1. Properties and van Genuchten Parameters of Select Soil Types.

Soil Type	Permeability	Density	Porosity		van Genuchten	
	$\kappa \text{ (m}^2\text{)}$	$\rho \text{ (kg/m}^3\text{)}$	θ_t	θ_r	α	m
Sand	9.9×10^{-12}	1430	0.38	5.3×10^{-2}	3.5	3.2
Loamy Sand	1.6×10^{-12}	1430	0.39	4.9×10^{-2}	3.5	1.7
Sandy Loam	5.9×10^{-13}	1460	0.39	3.9×10^{-2}	2.7	1.4
Sandy Clay Loam	2.0×10^{-13}	1430	0.38	6.3×10^{-2}	2.1	1.3
Loam	1.9×10^{-13}	1380	0.40	6.1×10^{-2}	1.5	1.5
Silt Loam	2.8×10^{-13}	1380	0.44	6.5×10^{-2}	0.51	1.7
Clay Loam	1.3×10^{-13}	1500	0.44	7.9×10^{-2}	1.6	1.4
Silt Clay Loam	1.7×10^{-13}	1390	0.48	9.0×10^{-2}	0.84	1.5
Silt Clay	1.5×10^{-13}	1300	0.48	1.1×10^{-1}	1.6	1.3
Silt	6.7×10^{-13}	1260	0.49	5.0×10^{-2}	0.66	1.7
Sandy Clay	1.7×10^{-13}	1470	0.39	1.2×10^{-1}	3.3	1.2
Clay	2.3×10^{-13}	1330	0.46	9.8×10^{-2}	1.3	1.3
Gravel	1.3×10^{-9}	1430	0.42	5.0×10^{-3}	100	2.19